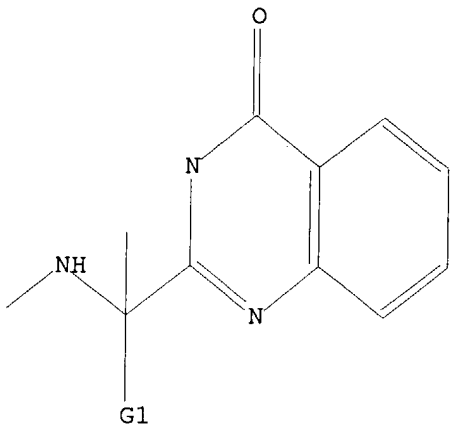


G1 C,H

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss full
FULL SEARCH INITIATED 14:33:37 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 44607 TO ITERATE

100.0% PROCESSED 44607 ITERATIONS 234 ANSWERS
SEARCH TIME: 00.00.04

L2 234 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	155.42	155.63

FILE 'CAPLUS' ENTERED AT 14:33:46 ON 14 SEP 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 14 Sep 2004 VOL 141 ISS 12
FILE LAST UPDATED: 13 Sep 2004 (20040913/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 12

L3 30 L2

=> d l3 1-30 ibib abs hitstr

L3 ANSWER 1 OF 30 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2004:589250 CAPLUS
DOCUMENT NUMBER: 141:140470
TITLE: Preparation of aminophenylbenzamides as inhibitors of histone deacetylase
INVENTOR(S): Delorme, Daniel; Zhou, Zhihong
PATENT ASSIGNEE(S): Methylgene, Inc., Can.
SOURCE: U.S. Pat. Appl. Publ., 318 pp., Cont.-in-part of U.S. Ser. No. 242,304.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004142953	A1	20040722	US 2003-358556	20030204
US 2004106599	A1	20040603	US 2002-242304	20020912
WO 2004069823	A1	20040819	WO 2004-CA139	20040204

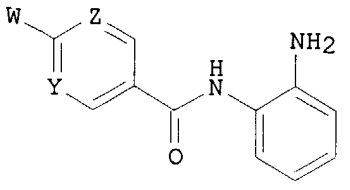
W: AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AZ, AZ, BA, BB, BG, BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO, CR, CR, CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG, ES, ES, FI, FI, GB, GD, GE, GE, GH, GM, HR, HR, HU, HU, ID, IL, IN, IS, JP, JP, KE, KE, KG, KG, KP, KP, KP, KR, KR, KZ, KZ, KZ, LC, LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN, MW, MX, MX, MZ, MZ, NA, NI
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:

US 2001-322402P	P	20010914
US 2002-391728P	P	20020626
US 2002-242304	A2	20020912
US 2003-358556	A	20030204

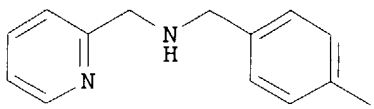
GI

date not good



I

Q^1 =



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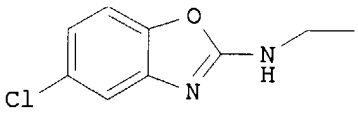

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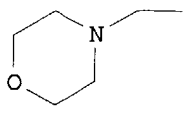


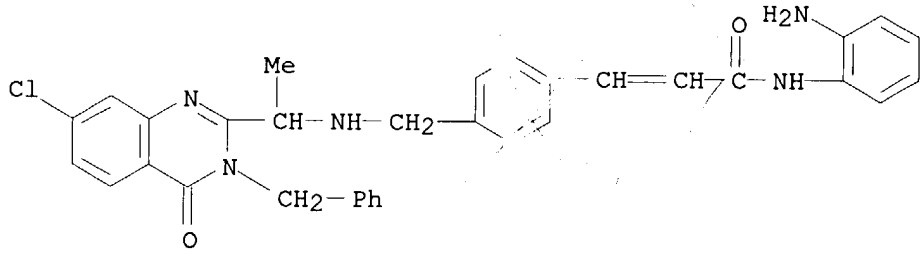
AB Title compds. e.g. (I; Y, Z = N, CH; W = Q1, Q2, Q3, etc.), were prepared

Thus, 4-[[(4-Amino-6-(2-indanylamino)-[1,3,5]triazin-2-yl)amino]methyl]benzoic acid (preparation given) in DMF was stirred with Et3N, BOP, and 1,2-phenylenediamine to give 63% 4-[[(4-Amino-6-(2-indanylamino)-[1,3,5]triazin-2-yl)amino]methyl]-N-(2-aminophenyl)benzamide. The latter inhibited human histone deacetylase HDAC-1 with IC50 = 0.4 μM.

IT **503041-91-6P**, N-(2-Aminophenyl)-3-(4-(((1-(3-benzyl-7-chloro-3,4-dihydro-4-oxoquinazolin-2-yl)ethyl)amino)methyl)phenyl)acrylamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of aminophenylbenzamides as inhibitors of histone deacetylase for treating cell proliferative disorders)

RN 503041-91-6 CAPLUS

CN 2-Propenamide, N-(2-aminophenyl)-3-[4-[[[1-[7-chloro-3,4-dihydro-4-oxo-3-(phenylmethyl)-2-quinazolinyl]ethyl]amino]methyl]phenyl]- (9CI) (CA INDEX NAME)



L3 ANSWER 2 OF 30 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2004:534196 CAPLUS

DOCUMENT NUMBER: 141:89125

TITLE: Preparation of oxodiazepanylquinazolinones as modulators of KSP kinesin activity for treatment of proliferative disease.

INVENTOR(S): Bergnes, Gustave; Dhanak, Dashyant; Knight, Steven David; Lu, Pu Ping; Morgans, David J., Jr.; Newlander, Kenneth Allen

PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA; Cytokinetics

SOURCE: PCT Int. Appl., 69 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

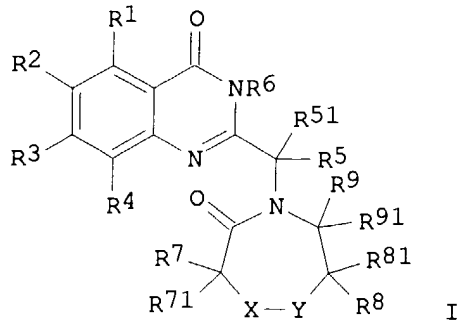
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004055008	A1	20040701	WO 2003-US39708	20031212

W: AE, AG, AL, AU, BA, BB, BR, BZ, CA, CN, CO, CR, CU, DM, DZ, EC, EG, GD, GE, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MA, MG, MK, MN, MX, NO, NZ, OM, PH, PL, RO, SC, SG, TN, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:		
US 2002-433494P	P	20021213
US 2002-435001P	P	20021219

OTHER SOURCE(S): MARPAT 141:89125
GI



I

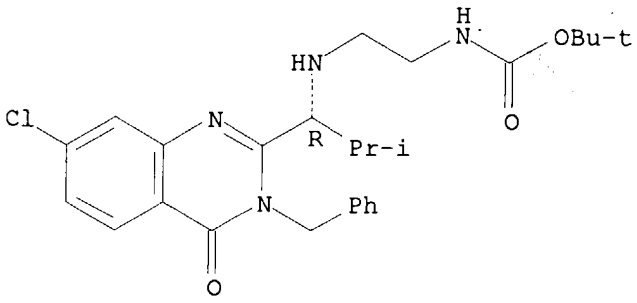
AB Title compds. [I; R1-R4 = H, halo, OH, NO2, cyano, (substituted) alkyl, alkoxy, aryl, heteroaryl, etc.; R5, R51 = H, (substituted) alkyl, aryl, aralkyl, heteroaryl, heteroaralkyl; R5R51C = 3-7 membered carbocyclyl; R6 = H, (substituted) alkyl, aryl, aralkylo, heteroaryl, heteroaralkyl; R7, R71, R8, R81, R9, R91 = H, (substituted) alkyl, aryl, aralkyl, heteroaryl, heteroaralkyl; X, Y = CR10R11, NR12, O, S; R10, R11 = H, (substituted) alkyl, aryl, heteroaryl; R12 = H, (substituted) alkyl, aralkyl, heteroaralkyl, alkylcarbonyl, arylcarbonyl, heteroarylcarbonyl, aralkylcarbonyl, heteroaralkylcarbonyl, alkoxycarbonyl, etc.], were prepared Thus, N-(2-aminoethyl)-N-[1-(3-benzyl-7-chloro-4-oxo-3,4-dihydroquinazolin-2-yl)-2-methylpropyl]acrylamide (preparation given) was refluxed overnight in MeOH to give 3-benzyl-7-chloro-2-[2-methyl-1-(7-oxo-1,4-diazepan-1-yl)propyl]-3H-quinazolin-4-one. Some I inhibited cell proliferation with GI50 <10 nM.

IT **713526-39-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of oxodiazepanylquinazolinones as modulators of KSP kinesin activity)

RN 713526-39-7 CAPLUS

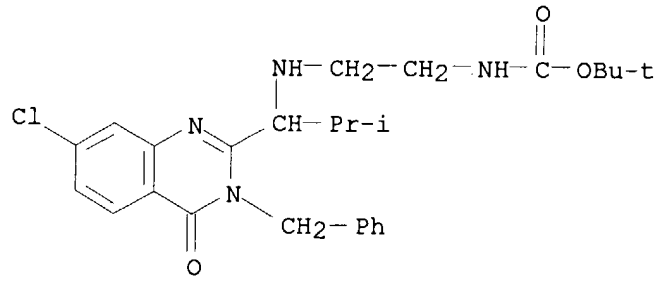
CN Carbamic acid, [2-[[(1R)-1-[7-chloro-3,4-dihydro-4-oxo-3-(phenylmethyl)-2-quinazolinyl]-2-methylpropyl]amino]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

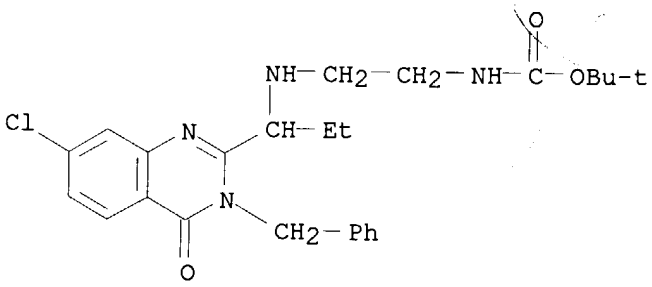


IT **713526-27-3P 713526-34-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of oxodiazepanylquinazolinones as modulators of KSP kinesin

activity)
RN 713526-27-3 CAPLUS
CN Carbamic acid, [2-[[1-[7-chloro-3,4-dihydro-4-oxo-3-(phenylmethyl)-2-quinazolinyl]-2-methylpropyl]amino]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 713526-34-2 CAPLUS
CN Carbamic acid, [2-[[1-[7-chloro-3,4-dihydro-4-oxo-3-(phenylmethyl)-2-quinazolinyl]propyl]amino]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 30 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2004:80465 CAPLUS
DOCUMENT NUMBER: 140:139471
TITLE: Preparation of of quinazolinone-like derivatives to treat cellular proliferative diseases
INVENTOR(S): Bergnes, Gustave; Smith, Whitney W.; Yao, Bing; Morgans, David J., Jr.; MacDonald, Andrew
PATENT ASSIGNEE(S): Cytokinetics, Inc., USA
SOURCE: PCT Int. Appl., 64 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004009036	A2	20040129	WO 2003-US23319	20030723
WO 2004009036	A3	20040819		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,

CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2004142949 A1 20040722 US 2003-626012 20030723

PRIORITY APPLN. INFO.: US 2002-398224P P 20020723

OTHER SOURCE(S): MARPAT 140:139471

AB The invention relates to quinazolinone-like derivs. that are inhibitors of the mitotic kinesin KSP and are useful in the treatment of cellular proliferative diseases, for example cancer, hyperplasias, restenosis, cardiac hypertrophy, immune disorders and inflammation. Preparation of 3-Benzyl-7-chloro-2-(3-benzyl-2-oxohexahydropyrimidin-4-yl)-3H-quinazolin-4-one is included.

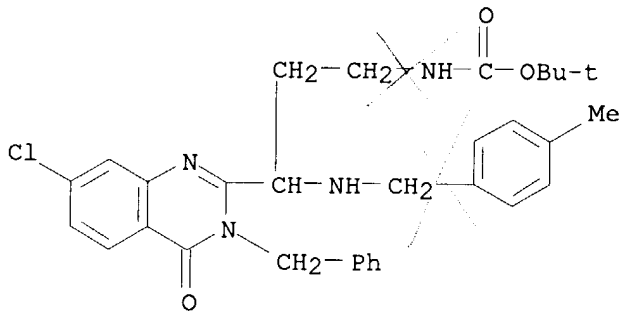
IT **651323-47-6P 651323-48-7P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of quinazolinone derivs. to treat cellular proliferative diseases)

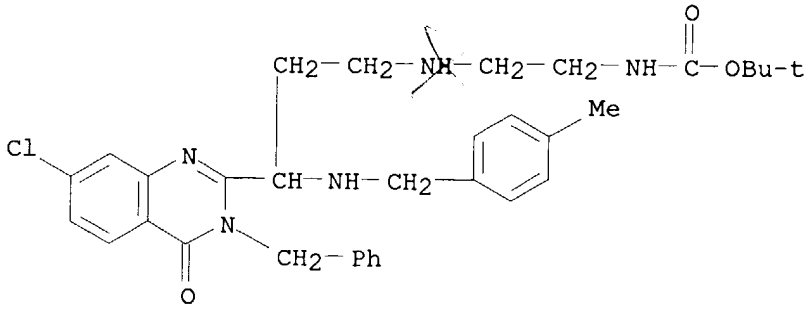
RN 651323-47-6 CAPLUS

CN Carbamic acid, [3-[7-chloro-3,4-dihydro-4-oxo-3-(phenylmethyl)-2-quinazolinyl]-3-[[(4-methylphenyl)methyl]amino]propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 651323-48-7 CAPLUS

CN Carbamic acid, [2-[[3-[7-chloro-3,4-dihydro-4-oxo-3-(phenylmethyl)-2-quinazolinyl]-3-[[(4-methylphenyl)methyl]amino]propyl]amino]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 4 OF 30 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:1006962 CAPLUS
DOCUMENT NUMBER: 140:59652
TITLE: Preparation of fused-ring pyrimidin-4(3H)-one derivatives as LXR modulators
INVENTOR(S): Kaneko, Satoru; Watanabe, Tsuyoshi; Oda, Kozo; Mohan, Raju; Schweiger, Edwin J.; Martin, Richard
PATENT ASSIGNEE(S): Sankyo Company, Limited, Japan; X-Ceptor Therapeutics, Inc.
SOURCE: PCT Int. Appl., 465 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003106435	A1	20031224	WO 2003-JP7677	20030617

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2002-389662P P 20020618
OTHER SOURCE(S): MARPAT 140:59652
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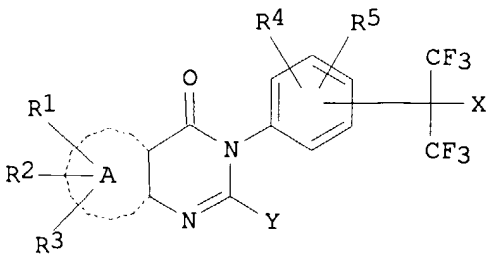
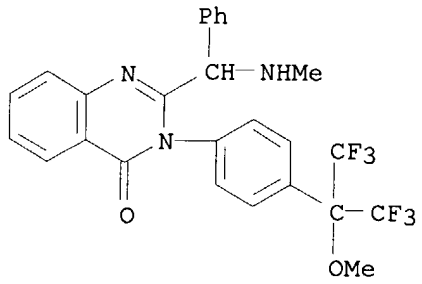


I

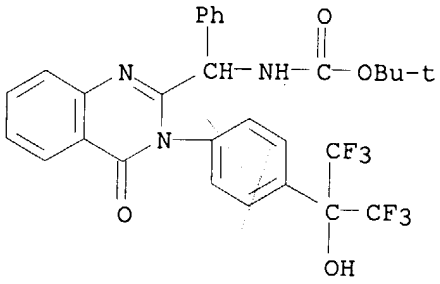
AB The title compds. [I; A = aryl or heteroaryl; R1-R3 = H, OH, NO2, CN, etc.; or R1 and R2 together = alkylenedioxy; R4, R5 = H, OH, NH2, halo, etc.; X = H, OH, halo, alkoxy, haloalkoxy; Y = (un)substituted alkyl, cycloalkyl, heterocyclyl, aryl, cycloalkylalkyl, heterocyclylalkyl or aralkyl] which can modulate LXR function and as a result show excellent anti-arteriosclerotic and anti-inflammatory activity, were prepared and formulated. Thus, reacting anthranilic acid with phenylacetic acid in the presence of PPh3 in pyridine followed by addition of 2-(4-aminophenyl)-1,1,1,3,3,3-hexafluoro-2-propanol afforded 76% 2-benzyl-3-{4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl}-4(3H)-quinazolinone.

The compds. I showed excellent binding affinity against LXR (biol. data were given).

IT **637345-89-2P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of fused-ring pyrimidin-4(3H)-one derivs. as LXR modulators)
RN 637345-89-2 CAPLUS
CN 4(3H)-Quinazolinone, 2-[(methylamino)phenylmethyl]-3-[4-[2,2,2-trifluoro-1-methoxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



IT **637347-68-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of fused-ring pyrimidin-4(3H)-one derivs. as LXR modulators)
RN 637347-68-3 CAPLUS
CN Carbamic acid, [[3,4-dihydro-4-oxo-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-2-quinazolinyl]phenylmethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 5 OF 30 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:931177 CAPLUS
DOCUMENT NUMBER: 140:5063
TITLE: 2-[1-(Imidazol-1-yl)alkyl]-3H-quinazolin-4-one derivatives, pharmaceutical compositions containing them, and methods of their use as KSP kinesin inhibitors for the treatment of cellular proliferative diseases
INVENTOR(S): Feng, Bainian; Bergnes, Gustave; Morgans, David J. C., Jr.; Dhanak, Dashyant; Knight, Steven David; Darcy, Michael Gerard

PATENT ASSIGNEE(S): Cytokinetics, Inc., USA; Smithkline Beecham Corporation
SOURCE: PCT Int. Appl., 97 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003097053	A1	20031127	WO 2003-US14787	20030508
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
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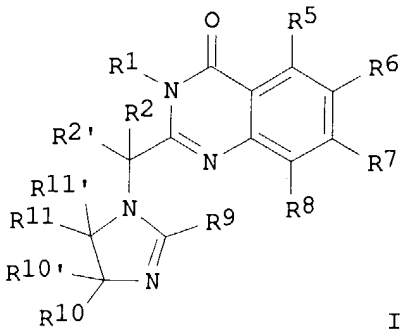
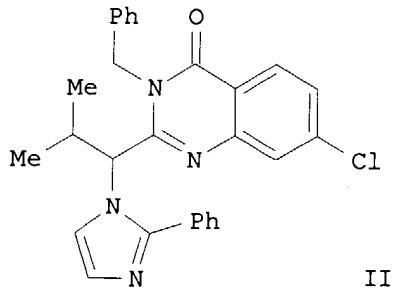
US 2004077668	A1	20040422	US 2003-435069	20030508

PRIORITY APPLN. INFO.: US 2002-379531P P 20020509
OTHER SOURCE(S): MARPAT 140:5063
GI



I



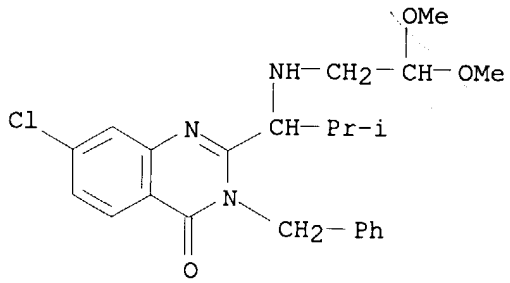
II

AB Compds. useful for treating cellular proliferative diseases and disorders by modulating the activity of KSP (kinesin-like spindle protein), and especially human KSP, are disclosed (no data). In particular, compds. I are claimed [wherein: R1 = H, (un)substituted alkyl, aryl, aralkyl, heteroaryl, or heteroaralkyl; R2, R2' = H, (un)substituted alkyl, aryl, aralkyl, heteroaryl, or heteroaralkyl; or R2R2' = (un)substituted 3- to 7-membered ring; R5, R6, R7, R8 = H, (un)substituted alkyl or alkoxy, halo, OH, NO2, cyano, dialkylamino, alkylsulfonyl, alkylsulfonamido, alkylthio, carboxyalkyl, carboxamido, aminocarbonyl, (un)substituted aryl, aryloxy, heteroaryl, or heteroaryloxy; R9 = H, (un)substituted alkyl, aryl, aralkyl, or heteroaryl; R10, R10', R11, R11' = H, (un)substituted alkyl, aryl, or aralkyl; or R10'R11' = pi bond; including single and mixed stereoisomers and pharmaceutically acceptable salts and/or solvates].

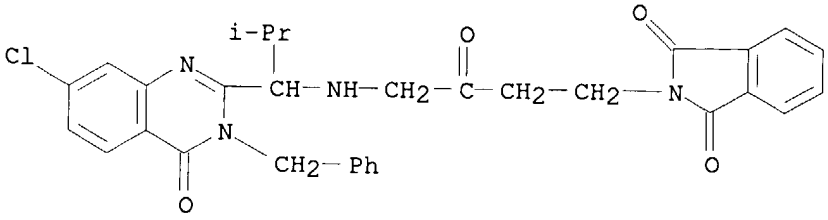
Approx. 60 compds. I are described in examples. Compds. I having (R)-configuration at the stereogenic center bearing R2 are preferred for reasons of greater potency than the (S)-isomers. For instance, 2-(1-amino-2-methylpropyl)-3-benzyl-7-chloro-3H-quinazolin-4-one underwent a sequence of N-alkylation at amino with BrCH2CH(OMe)2 and K2CO3 (59%), amidation of the resultant secondary amine with PhCOCl and Et3N (54%), and deprotection/cyclocondensation with NH4OAc in refluxing AcOH (23%) to give invention compound II. Compds. I are said to be active against human ovarian cancer cells SKOV3 in vitro. Visual inspection revealed that the compds. caused cell cycle arrest in the prometaphase stage of mitosis; DNA was condensed and spindle formation had initiated, but arrested cells uniformly displayed monopolar spindles, indicating that there was an inhibition of spindle pole body separation

IT **627891-88-7P 627891-90-1P 627891-92-3P**
627891-93-4P 627891-94-5P 627891-95-6P
627892-04-0P 627892-10-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of (imidazolylalkyl)quinazolinone derivs. as KSP kinesin inhibitors for the treatment of cellular proliferative diseases)

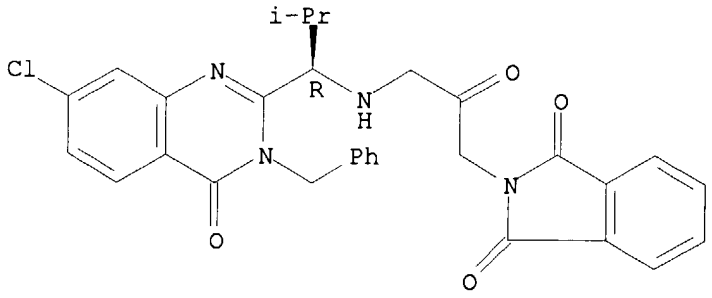
RN 627891-88-7 CAPLUS
CN 4(3H)-Quinazolinone, 7-chloro-2-[1-[(2,2-dimethoxyethyl)amino]-2-methylpropyl]-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 627891-90-1 CAPLUS
CN 1H-Isoindole-1,3(2H)-dione, 2-[4-[[1-[7-chloro-3,4-dihydro-4-oxo-3-(phenylmethyl)-2-quinazolinyl]-2-methylpropyl]amino]-3-oxobutyl]- (9CI) (CA INDEX NAME)

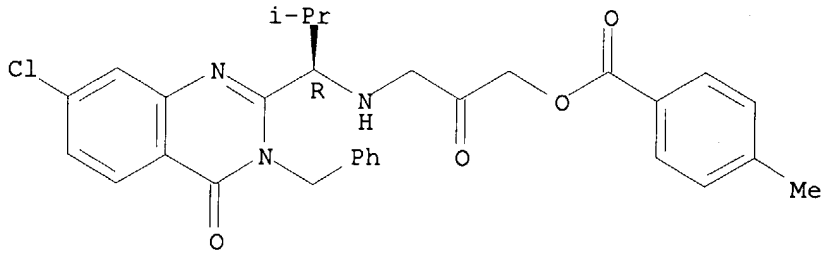


RN 627891-92-3 CAPLUS
CN Carbamic acid, [2-[[1-[7-chloro-3,4-dihydro-4-oxo-3-(phenylmethyl)-2-quinazolinyl]-2-methylpropyl]amino]-1,1-dimethylethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



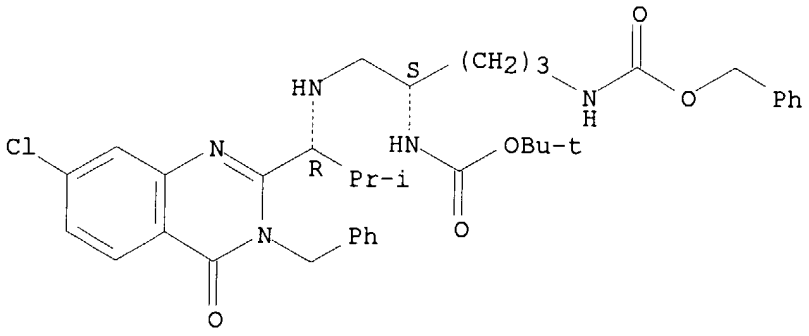
RN 627892-04-0 CAPLUS
CN Benzoic acid, 4-methyl-, 3-[[(1R)-1-[7-chloro-3,4-dihydro-4-oxo-3-(phenylmethyl)-2-quinazolinyl]-2-methylpropyl]amino]-2-oxopropyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 627892-10-8 CAPLUS
CN Carbamic acid, [(4S)-5-[[(1R)-1-[7-chloro-3,4-dihydro-4-oxo-3-(phenylmethyl)-2-quinazolinyl]-2-methylpropyl]amino]-4-[[(1,1-dimethylethoxy)carbonyl]amino]pentyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

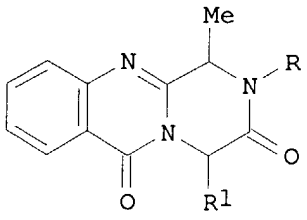
Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 6 OF 30 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:773476 CAPLUS
DOCUMENT NUMBER: 141:23488
TITLE: A preparation of pyrazino[2,1-b]quinazolone derivatives useful as multidrug resistance modulators

AUTHOR(S): Kokosi, Jozsef; Almasi, Janos; Podanyi, Benjamin; Hermecz, Istvan
CORPORATE SOURCE: Gyogyszereszi Kemiai Intezet, Semmelweis Egyetem, Budapest, Russia
SOURCE: Acta Pharmaceutica Hungarica (2003), 73(1), 29-39
CODEN: APHGAO; ISSN: 0001-6659
PUBLISHER: Magyar Gyogyszereszeti Tarsasag
DOCUMENT TYPE: Journal
LANGUAGE: Hungarian
GI



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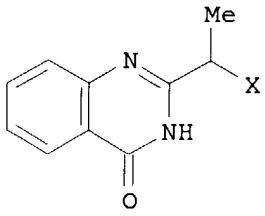


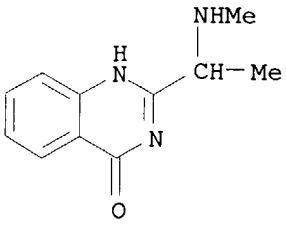
II

another date only good

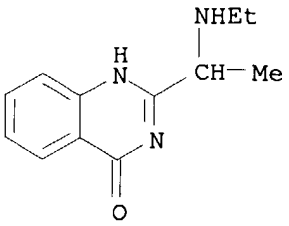
AB An exploration for new MDR-modulators utilizing pyrazino[2,1-b]quinazolones as scaffolds disclosed after systematic synthetic investigation highly hydrophobic N-substituted derivs. as readily accessible active tricyclic compds. (no biol. data). A versatile synthesis of 2-substituted-1,2,3,4-tetrahydro-6H-pyrazino[2,1-b]quinazoline-3,6-diones is presented starting from 2,3-substituted quinazolones. The new compds. have been characterized by elemental analyses, NMR, and in some cases by 13C ruler, and X-ray investigations. For instance, pyrazino[2,1-b]quinazoline derivative I was prepared via amination of quinazoline II (X = Br) by RNH2, N-acetylation of the obtained amine II (X = NHR) by YCH(R1)C(O)Y (R1 is H or Me; Y is Cl or Br), and subsequent heterocyclization of the obtained amide II [X = N(R)C(O)C(Y)R1].

IT **143993-15-1P 143993-16-2P 143993-17-3P**
143993-18-4P 143993-20-8P 143993-21-9P
216596-07-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of pyrazino[2,1-b]quinazolone derivs. useful as multidrug resistance modulators)

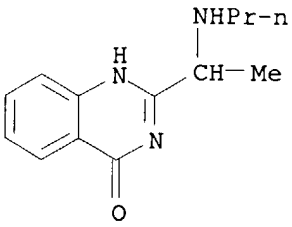
RN 143993-15-1 CAPLUS
CN 4(1H)-Quinazolinone, 2-[1-(methylamino)ethyl]- (9CI) (CA INDEX NAME)



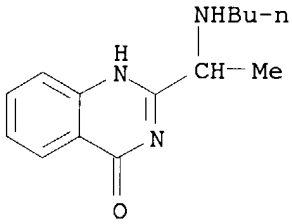
RN 143993-16-2 CAPLUS
CN 4(1H)-Quinazolinone, 2-[1-(ethylamino)ethyl]- (9CI) (CA INDEX NAME)



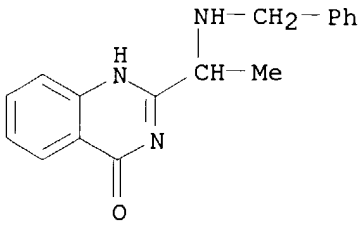
RN 143993-17-3 CAPLUS
CN 4(1H)-Quinazolinone, 2-[1-(propylamino)ethyl]- (9CI) (CA INDEX NAME)



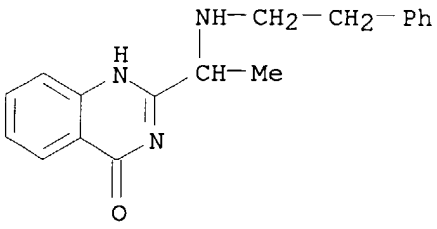
RN 143993-18-4 CAPLUS
CN 4(1H)-Quinazolinone, 2-[1-(butylamino)ethyl]- (9CI) (CA INDEX NAME)



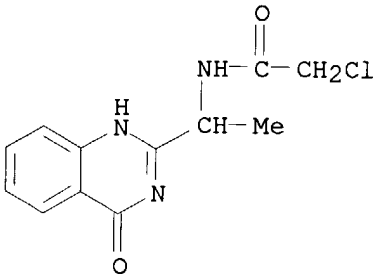
RN 143993-20-8 CAPLUS
CN 4(1H)-Quinazolinone, 2-[1-[(phenylmethyl)amino]ethyl]- (9CI) (CA INDEX NAME)



RN 143993-21-9 CAPLUS
CN 4(1H)-Quinazolinone, 2-[1-[(2-phenylethyl)amino]ethyl]- (9CI) (CA INDEX NAME)



RN 216596-07-5 CAPLUS
CN Acetamide, 2-chloro-N-[1-(1,4-dihydro-4-oxo-2-quinazolinyl)ethyl]- (9CI) (CA INDEX NAME)



L3 ANSWER 7 OF 30 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:772642 CAPLUS
DOCUMENT NUMBER: 140:380763
TITLE: Enantioseparation of quinazolone derivatives using an AGP-based liquid chromatography stationary phase
AUTHOR(S): Gyimesine Forras, Krisztina; Gergely, Andras; Kokosi, Jozsef
CORPORATE SOURCE: Gyogyszereszi Kemiai Intezet, Semmelweis Egyetem, Budapest, Hung.
SOURCE: Acta Pharmaceutica Hungarica (2003), 73(1), 5-12
CODEN: APHGAO; ISSN: 0001-6659
PUBLISHER: Magyar Gyogyszereszeti Tarsasag
DOCUMENT TYPE: Journal
LANGUAGE: Hungarian

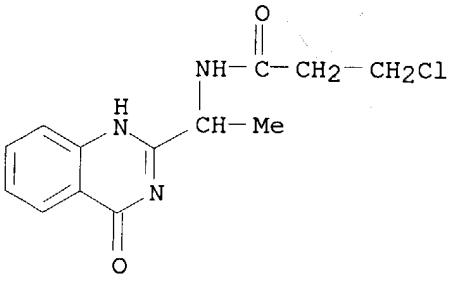
AB An AGP-based chiral stationary phase has been applied successfully for enantiosepn. of 4(3H)-quinazolone derivs. Chiral-AGP is proved to be an excellent selector, as optimized chromatog. conditions allow with one exception baseline resolution for the enantiomers of the potential cholecystokinin antagonist compds. (α=1.19-1.85). Retention and enantioselectivity could be modified to a large extent by varying the eluent pH and adding organic solvents with different types i.e. acetonitrile and 2-propanol to the buffered mobile phase. It was established that by increasing the eluent pH from 6.0 to 7.0 the retention factors of the model compds. bearing no protonable groups are increased in the presence of 7 volume/volume % (1.33 M) acetonitrile. However further increasing the acetonitrile content up to 10 volume/volume % or addition of 2-propanol in equimolar concentration (1.33 M) no similar changes could be detected with the same modification in the eluent pH. These observations are explained by changes in the sorption properties of the selector determined simultaneously by the type and concentration of organic modifier and also the eluent pH. The exptl. data give further insight into the chromatog. mechanism on a Chiral-AGP

column.

IT **172420-43-8**
RL: ANT (Analyte); ANST (Analytical study)
(enantiosepn. of quinazolone derivs. using an AGP-based liquid chromatog. stationary phase)

RN 172420-43-8 CAPLUS

CN Propanamide, 3-chloro-N-[1-(1,4-dihydro-4-oxo-2-quinazolinyl)ethyl]- (9CI) (CA INDEX NAME)



L3 ANSWER 8 OF 30 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:737738 CAPLUS

DOCUMENT NUMBER: 139:261313

TITLE: Quinazolinone amide compounds as modulators of nuclear receptors, particularly farnesoid X receptor (FXR) and/or orphan nuclear receptors, and their preparation, pharmaceutical compositions, and methods of use

INVENTOR(S): Martin, Richard; Kahl, Jeffery Dean; Flatt, Brenton Todd; Griffith, Ronald

PATENT ASSIGNEE(S): X-Ceptor Therapeutics, Inc., USA

SOURCE: PCT Int. Appl., 204 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003076418	A1	20030918	WO 2003-US6793	20030304

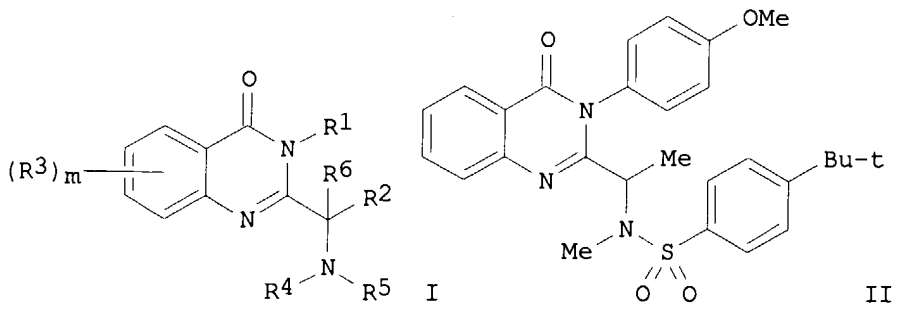
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2002-363132P P 20020307

OTHER SOURCE(S): MARPAT 139:261313

GI



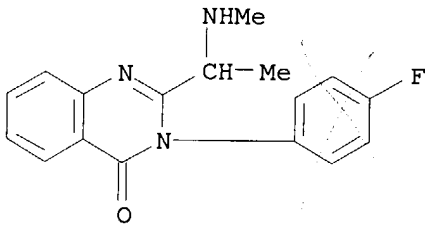
I II

AB Compds., pharmaceutical compns., and methods for modulating the activity of nuclear receptors are provided. In particular, amide-containing quinazolinones are provided for modulating the activity of farnesoid X receptor (FXR) and/or orphan nuclear receptors. The disclosed compds. include I [m = 0-4; R1 = H, (un)substituted alk(en/yn)yl, (hetero)aryl, cycloalkyl(alkyl), (hetero)aralkyl, heterocyclyl(alkyl) (preceding groups designated as group A), OH or derivs., NH2 or derivs.; R2, R6 = (independently) group A, or R2R6 = (un)substituted alkylene; R4, R5 = (independently) group A, OH or derivs, NH2 or derivs., various acyl, sulfinyl, sulfonyl, or phosphoryl groups, etc.; or R4R5 (un)substituted alkylene, alkenylene, alkenylene(oxy/aza)alkenylene; or any of R2R5, R2R4, R5R6, or R4R6 form 4- to 7-membered, (un)substituted heteroaryl or heterocyclyl group; R3 = (independently) halo, pseudohalo, group A, NH2 or derivs., OH or derivs., SH or derivs., various acyl, thioacyl, imidoyl, sulfinyl, or sulfonyl groups; or adjacent R3R3 = (un)substituted alkylene, alkenylene, alkylenedioxy, thioalkylenoxy, alkylenedithioxy; including stereoisomers, racemates, mixts., and pharmaceutically acceptable derivs.; with one exception compound]. Over 300 specific compds. were prepared and claimed by name. Ten of the most preferred compds. are named. The compds. are useful for treating diseases and disorders selected from: hypercholesterolemia, hyperlipoproteinemia, hypertriglyceridemia, lipodystrophy, hyperglycemia, diabetes mellitus, dyslipidemia, atherosclerosis, gallstone disease, acne vulgaris, acneiform skin conditions, diabetes, Parkinson's disease, cancer, Alzheimer's disease, inflammation, immunol. disorders, lipid disorders, obesity, conditions characterized by a perturbed epidermal barrier function, hyperlipidemia, cholestasis, peripheral occlusive disease, ischemic stroke, obesity, disease states associated with elevated cholesterol levels, conditions of disturbed differentiation or excess proliferation of the epidermis or mucous membrane, and cardiovascular disorders. For instance, Me anthranilate was N-amidated with 2-chloropropionyl chloride (97%), followed by saponification of the ester (97%), and amidation/cyclocondensation of the resultant acid using p-anisidine and PCl3 (72%), to give 2-(1-chloroethyl)-3-(4-methoxyphenyl)-3H-quinazolin-4-one. This intermediate chloride was aminated with methylamine in THF (99%), and the obtained secondary amine was sulfonylated with 4-tert-butylbenzenesulfonyl chloride and TEA in DCM (92%), to give preferred invention compound II. In an FRET assay for binding to human FXR (ligand-binding domain, fused to glutathione-S-transferase), II had an EC50 of about 300 nM. In an FXR/ECREx7 co-transfection assay using African green monkey kidney cells, II had an efficacy of 190% relative to high control (chenodeoxycholic acid).

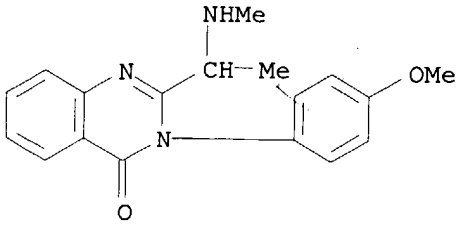
IT **330796-26-4P**, 3-(4-Fluorophenyl)-2-(1-methylaminoethyl)-3H-

quinazolin-4-one **602318-84-3P**, 3-(4-Methoxyphenyl)-2-(1-methylaminoethyl)-3H-quinazolin-4-one **602318-85-4P**, 2-(1-Methylaminoethyl)-3-p-tolyl-3H-quinazolin-4-one **602318-86-5P**, 6-Bromo-2-(1-methylaminoethyl)-3-p-tolyl-3H-quinazolin-4-one **602318-87-6P**, 3-(2,4-Dimethylphenyl)-2-(1-methylaminoethyl)-3H-quinazolin-4-one **602318-89-8P**, 3-(4-Methoxyphenyl)-8-methyl-2-(1-methylaminoethyl)-3H-quinazolin-4-one **602318-90-1P**, 3-(4-Methoxyphenyl)-6-methyl-2-(1-methylaminoethyl)-3H-quinazolin-4-one **602318-91-2P**, 3-(4-Methoxyphenyl)-7-methyl-2-(1-methylaminoethyl)-3H-quinazolin-4-one **602318-92-3P**, 8-Methoxy-3-(4-methoxyphenyl)-2-(1-methylaminoethyl)-3H-quinazolin-4-one **602318-93-4P**, 5-Methoxy-3-(4-methoxyphenyl)-2-(1-methylaminoethyl)-3H-quinazolin-4-one **602318-94-5P**, 6-Methoxy-3-(4-methoxyphenyl)-2-(1-methylaminoethyl)-3H-quinazolin-4-one **602318-98-9P**, 3-(4-Bromophenyl)-2-(1-methylaminoethyl)-3H-quinazolin-4-one **602318-99-0P**, 2-(1-Methylaminoethyl)-3-phenyl-3H-quinazolin-4-one **602319-00-6P**, 3-(4-Chlorophenyl)-2-(1-methylaminoethyl)-3H-quinazolin-4-one **602319-01-7P**, 3-(3,5-Dimethylphenyl)-2-(1-methylaminoethyl)-3H-quinazolin-4-one **602319-02-8P**, 3-(4-Dimethylamino-phenyl)-2-(1-methylaminoethyl)-3H-quinazolin-4-one
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(intermediate and drug candidate; preparation of quinazolinone amides as farnesoid X and/or orphan nuclear receptor modulators)

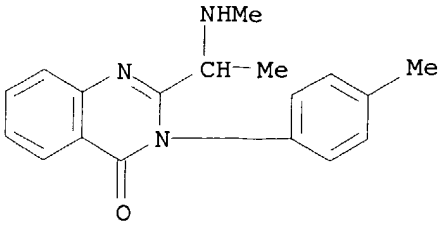
RN 330796-26-4 CAPLUS
CN 4(3H)-Quinazolinone, 3-(4-fluorophenyl)-2-[1-(methylamino)ethyl]- (9CI) (CA INDEX NAME)



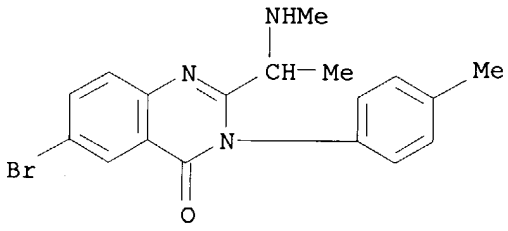
RN 602318-84-3 CAPLUS
CN 4(3H)-Quinazolinone, 3-(4-methoxyphenyl)-2-[1-(methylamino)ethyl]- (9CI) (CA INDEX NAME)



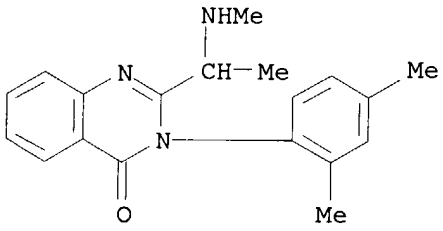
RN 602318-85-4 CAPLUS
CN 4(3H)-Quinazolinone, 2-[1-(methylamino)ethyl]-3-(4-methylphenyl)- (9CI) (CA INDEX NAME)



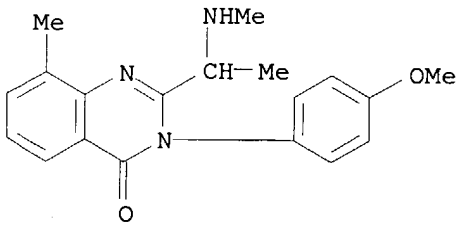
RN 602318-86-5 CAPLUS
CN 4(3H)-Quinazolinone, 6-bromo-2-[1-(methylamino)ethyl]-3-(4-methylphenyl)-
(9CI) (CA INDEX NAME)



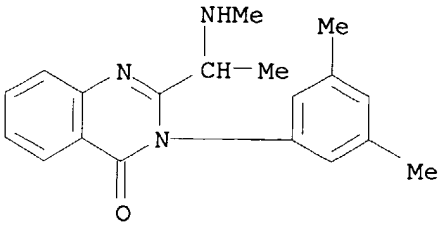
RN 602318-87-6 CAPLUS
CN 4(3H)-Quinazolinone, 3-(2,4-dimethylphenyl)-2-[1-(methylamino)ethyl]-
(9CI) (CA INDEX NAME)



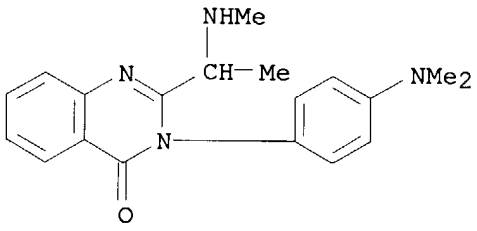
RN 602318-89-8 CAPLUS
CN 4(3H)-Quinazolinone, 3-(4-methoxyphenyl)-8-methyl-2-[1-(methylamino)ethyl]-
(9CI) (CA INDEX NAME)



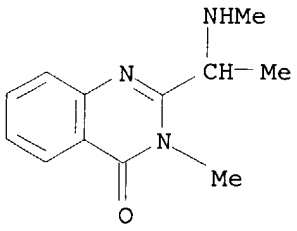
RN 602318-90-1 CAPLUS
CN 4(3H)-Quinazolinone, 3-(4-methoxyphenyl)-6-methyl-2-[1-(methylamino)ethyl]-
(9CI) (CA INDEX NAME)



RN 602319-02-8 CAPLUS
CN 4(3H)-Quinazolinone, 3-[4-(dimethylamino)phenyl]-2-[1-(methylamino)ethyl]- (9CI) (CA INDEX NAME)



IT **602318-96-7**, 3-Methyl-2-(1-methylaminoethyl)-3H-quinazolin-4-one
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of quinazolinone amides as farnesoid X and/or orphan nuclear receptor modulators)
RN 602318-96-7 CAPLUS
CN 4(3H)-Quinazolinone, 3-methyl-2-[1-(methylamino)ethyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 9 OF 30 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:678784 CAPLUS
DOCUMENT NUMBER: 139:214481
TITLE: Syntheses of enantiomerically pure quinazolinones
INVENTOR(S): Bergnes, Gustav; Ha, Edward; Yiannikourous, George; Kalaritis, Panos; Yonce, Brandon E.; Welday, Kurt Alan, Jr.
PATENT ASSIGNEE(S): Cytokinetics, Inc., USA; SmithKline Beecham Corp.
SOURCE: PCT Int. Appl., 59 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003070701	A2	20030828	WO 2003-US4713	20030214
WO 2003070701	A3	20031016		
WO 2003070701	B1	20031218		

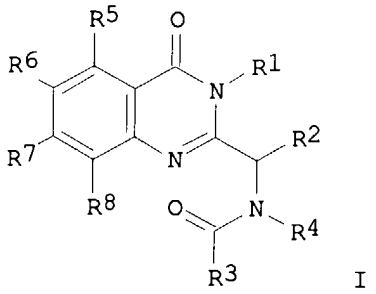
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2004067969	A1	20040408	US 2003-366828		20030214
PRIORITY APPLN. INFO.:			US 2002-357244P	P	20020215
			US 2002-380746P	P	20020514

OTHER SOURCE(S): MARPAT 139:214481

GI



I

AB The present invention provides intermediates, synthetic methods and novel quinazolinone (shown as I; e.g. (R)-N-(3-aminopropyl)-N-[1-(3-benzyl-7-chloro-4-oxo-3,4-dihydroquinazolin-2-yl)-2-methylpropyl]-4-methylbenzamide) compns. of matter, which are inhibitors of the mitotic kinesin KSP (no data) and are useful in the treatment of cellular proliferative diseases, for example cancer, hyperplasias, restenosis, cardiac hypertrophy, immune disorders and inflammation (no data); only the compds., compns. of matter and synthetic methods are claimed. The method comprises contacting HO2CCH(R2)NHX (R2 = oxaalkyl or (un)substituted alkyl, aryl, alkylaryl, heteroaryl, or alkylheteroaryl; X = H, protecting group (e.g. Boc, CBZ, phthalide, allyloxycarbonyl, 2,2,2-trichloroethoxycarbonyl); e.g. valine) with iso-Bu chloroformate followed by contacting the resulting product with (un)substituted 2-aminobenzoic acids to give I. Eight example prepns. of I are included. For example, (S)-[1-(3-benzyl-7-chloro-4-oxo-3,4-dihydroquinazolin-2-yl)-2-methylpropyl]carbamic acid tert-Bu ester was prepared starting from N-Boc-L-valine and involving intermediates 2-[[2-[(tert-butoxycarbonyl)amino]-L-3-methylbutyryl]amino]-4-chlorobenzoic acid, (S)-[1-(7-chloro-4-oxo-4H-benzo[d][1,3]oxazin-2-yl)-2-methylpropyl]carbamic acid tert-Bu ester, (S)-[1-[[(2-benzylcarbamoyl-5-

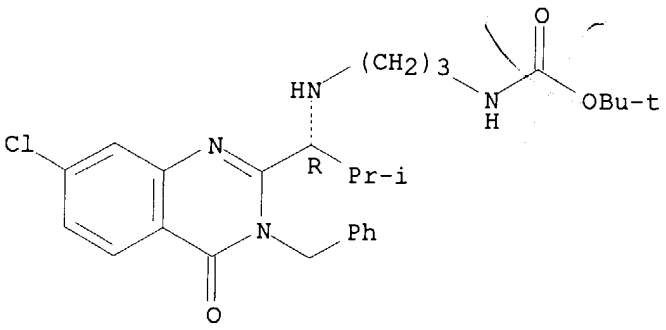
chlorophenyl)imino]methyl]-2-methylpropyl]carbamic acid tert-Bu ester (in mixture with the final product). In the key step, to 2-[[2-[(tert-butoxycarbonyl)amino]-L-3-methylbutyryl]amino]-4-chlorobenzoic acid was added 13.2 mL (0.1 mol) of iso-Bu chloroformate over 15 min (internal temperature 5°) followed by the addition of 11.1 mL (0.1 mol) of anhydrous N-methylmorpholine over 15 min at 0°; the mixture was stirred for an addnl. hour at 0° to give (S)-[1-(7-chloro-4-oxo-4H-benzo[d][1,3]oxazin-2-yl)-2-methylpropyl]carbamic acid tert-Bu ester. For I: R1 is H or (un)substituted alkyl, aryl, alkylaryl, heteroaryl, or alkylheteroaryl; R3 is H, oxaalkyl, R9O-, R9NH- or (un)substituted alkyl, aryl, alkylaryl, heteroaryl, alkylheteroaryl, or oxaalkylaryl; R4 is H or (un)substituted alkyl, aryl, alkylaryl, heteroaryl, or alkylheteroaryl; R5, R6, R7 and R8 = H, hydroxy, (un)substituted alkyl, alkoxy, halogen, fluoroalkyl, nitro, cyano, amino, alkylamino, dialkylamino, alkylsulfonyl, alkylsulfonamido, sulfonamidoalkyl, sulfonamidoaryl, alkylthio, carboxyalkyl, carboxamido, aminocarbonyl, aryl or heteroaryl; and R9 is (un)substituted alkyl, aryl, alkylaryl, heteroaryl, or alkylheteroaryl. The compns. of matter comprise I and detectable amts. of ≥1 unreacted starting materials and/or a cyclo-dehydration reagent; they are claimed, presumably because it is important to monitor the purity of pharmaceutical compds. for the presence of such materials, which presence comprises a way of detecting use of a process of the invention.

IT **587881-27-4P**, (R)-[3-[[1-(3-Benzyl-7-chloro-4-oxo-3,4-dihydroquinazolin-2-yl)-2-methylpropyl]amino]propyl]carbamic acid tert-butyl ester **587881-29-6P**, (S)-[1-(3-Benzyl-7-chloro-4-oxo-3,4-dihydroquinazolin-2-yl)-2-methylpropyl]carbamic acid tert-butyl ester **587881-33-2P**, (R)-[1-(3-Benzyl-7-chloro-4-oxo-3,4-dihydroquinazolin-2-yl)-2-methylpropyl]carbamic acid tert-butyl ester **587881-35-4P**, (S)-[1-(7-Chloro-4-oxo-3,4-dihydroquinazolin-2-yl)-2-methylpropyl]carbamic acid tert-butyl ester **587881-39-8P**, (R)-[1-(7-Chloro-4-oxo-3,4-dihydroquinazolin-2-yl)-2-methylpropyl]carbamic acid tert-butyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(syntheses of enantiomerically pure quinazolinones)

RN 587881-27-4 CAPLUS

CN Carbamic acid, [3-[[(1R)-1-[7-chloro-3,4-dihydro-4-oxo-3-(phenylmethyl)-2-quinazolinyl]-2-methylpropyl]amino]propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

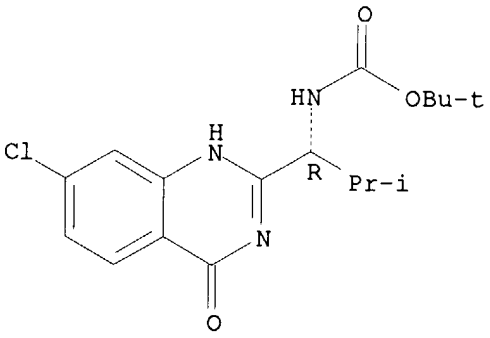


RN 587881-29-6 CAPLUS

CN Carbamic acid, [(1S)-1-[7-chloro-3,4-dihydro-4-oxo-3-(phenylmethyl)-2-quinazolinyl]-2-methylpropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

methylpropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



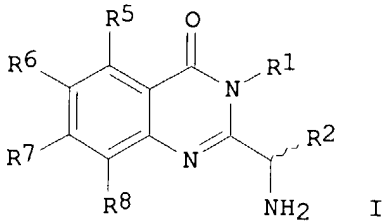
L3 ANSWER 10 OF 30 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:417728 CAPLUS
DOCUMENT NUMBER: 139:6884
TITLE: Process for the racemization of chiral quinazolinones
INVENTOR(S): Yao, Bing; Smith, Whitney W.; Bergnes, Gustave; Morgans, David, Jr.
PATENT ASSIGNEE(S): Cytokinetics, Inc., USA
SOURCE: PCT Int. Appl., 31 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003043995	A1	20030530	WO 2002-US37410	20021120
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003166933	A1	20030904	US 2002-300967	20021120
US 6753428	B2	20040622		

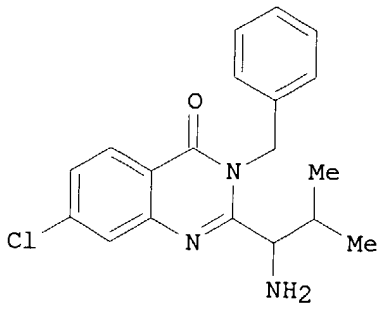
PRIORITY APPLN. INFO.: US 2001-332148P P 20011120
OTHER SOURCE(S): MARPAT 139:6884
GI

applicant

compounds - not claimed date not good



I



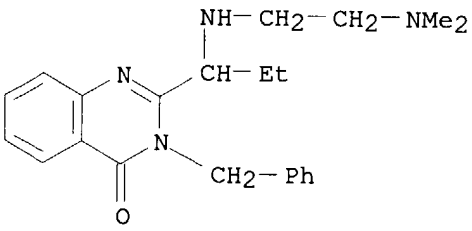
II

AB Racemates were obtained from one of the enantiomers, or an enantiomerically enriched mixture, of an optically active quinazolinone derivative I [wherein R1 = H or (un)substituted alkyl, (hetero)aryl, or (hetero)aralkyl; R2 = oxaalkyl or (un)substituted alkyl, (hetero)aryl, or (hetero)aralkyl; R5-R8 = independently H, (fluoro)alkyl, alkoxy, halo, NO2, dialkylamino, alkylsulfonyl, alkylsulfamido(alkyl), sulfonamidoaryl, alkylthio, carboxyalkyl, carboxamido, aminocarbonyl, or (hetero)aryl] by reaction of the compound with an alkali alkoxide of a primary alc. and isolation of the racemate. For example, treatment of (S)-II with NaOEt (21% by weight solution in denatured alc. containing 5% toluene) in absolute EtOH and heating at reflux for 36 h, followed by crystallization gave (±)-II in a 1:1.1 mixture of (R)- and (S)-isomers. The invention also provides for the subsequent resolution of the racemate and use of the other enantiomer in the synthesis of pharmacol. active therapeutic agents. Thus, an efficient method of converting an inactive or undesirable enantiomer into the other usable, desirable enantiomer is disclosed.

IT **336119-90-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation and racemization of chiral quinazolinones)

RN 336119-90-5 CAPLUS

CN 4(3H)-Quinazolinone, 2-[1-[[2-(dimethylamino)ethyl]amino]propyl]-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 11 OF 30 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:242160 CAPLUS

DOCUMENT NUMBER: 138:271705

TITLE: Preparation of triazinyl and other carboxamides as inhibitors of histone deacetylase

INVENTOR(S): Delorme, Daniel; Woo, Soon Hyung; Vaisburg, Arkadii; Moradel, Oscar; Leit, Silvana; Raeppel, Stephane;

PATENT ASSIGNEE(S): Frechette, Sylvie; Bouchain, Giliane
Methylgene, Inc., Can.
SOURCE: PCT Int. Appl., 347 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003024448	A2	20030327	WO 2002-US29017	20020912
WO 2003024448	A3	20031113		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

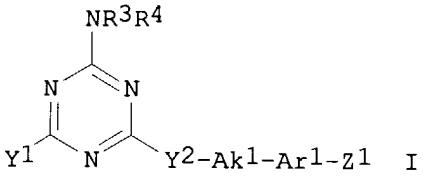
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1429765	A2	20040623	EP 2002-763627	20020912

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK

PRIORITY APPLN. INFO.:
US 2001-322402P P 20010914
US 2002-391728P P 20020626
WO 2002-US29017 W 20020912

OTHER SOURCE(S): MARPAT 138:271705
GI



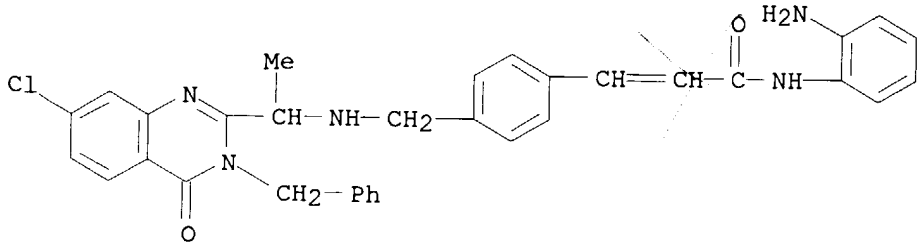
I

AB The invention relates to triazines (shown as I; variables defined below; e.g. 4-[[4-amino-6-(2-indanylamino)-[1,3,5]triazin-2-ylamino]methyl]-N-(2-aminophenyl)benzamide) and Cy3-X1-Ar2-(C(R5):C(R6))qC(O)NH-Ay2 (II; variables defined below; e.g.), many of which are N-(o-aminophenyl)carboxamides, as inhibitors of histone deacetylase (data included for many I and II). The invention provides compds. and methods for inhibiting histone deacetylase enzymic activity. The invention also provides compns. and methods for treating cell proliferative diseases and conditions. Antineoplastic effects of some I and II are illustrated for colorectal, pulmonary and pancreatic neoplasms; also the combined antineoplastic effect of histone deacetylase inhibitors and histone deacetylase antisense oligonucleotides on tumor cells in vivo was demonstrated. For I: R3 and R4 = H, L1, Cy1 and -L1-Cy1 (L1 = C1-C6 alkyl, C2-C6 heteroalkyl, or C3-C6 alkenyl; Cy1 = cycloalkyl, aryl, heteroaryl, or heterocyclyl) or R3 and R4 are taken together with the

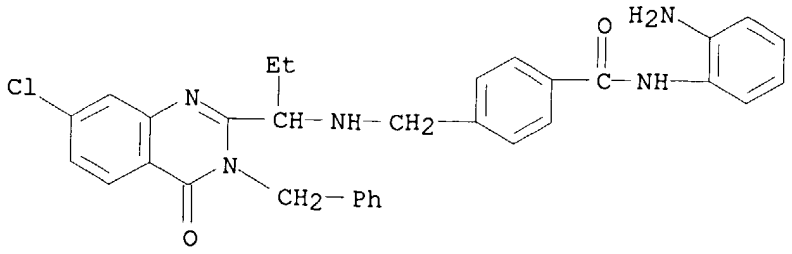
adjacent N atom to form a 5-, 6-, or 7-membered ring, wherein the ring atoms = C, O, S, and N, and wherein the ring is optionally substituted, and optionally forms part of a bicyclic ring system, or is optionally fused to one or two aryl or heteroaryl rings, or to one or two saturated or partially unsatd. cycloalkyl or heterocyclic rings, each of which rings and ring systems is optionally substituted. Y1 = -N(R1)(R2), -CH2-C(O)-N(R1)(R2), halogen, and H (R1 and R2 = H, L1, Cy1, and -L1-Cy1). Y2 = chemical bond or N(R0) (R0 = H, alkyl, aryl, aralkyl, and acyl); Ak1 = C1-C6 alkylene, C1-C6-heteroalkylene (preferably, in which one -CH2- is replaced with -NH-, and more preferably -NH-CH2), C2-C6 alkenylene or C2-C6 alkynylene; Ar1 = arylene or heteroarylene, either of which is optionally substituted; and Z1 = C(O)NH-Ay1 and CH:CHC(O)NH-Ay1 (Ay1 = aryl or heteroaryl, each of which is optionally substituted). For II: Cy2 = cycloalkyl, aryl, heteroaryl, or heterocyclyl; X1 = covalent bond, M1-L2-M1, and L2-M2-L2 (L2 = chemical bond, C1-C4 alkylene, C2-C4 alkenylene, and C2-C4 alkynylene, provided that L2 is not a chemical bond when X1 is M1-L2-M1; M1 = -O-, -N(R7)-, -S-, -S(O)-, S(O)2-, -S(O)2N(R7)-, -N(R7)S(O)2-, -C(O)-, -C(O)NH-, -NHC(O)-, -NHC(O)-O- and -OC(O)NH- (R7 = H, alkyl, aryl, aralkyl, acyl, heterocyclyl, and heteroaryl); and M2 = M1, heteroarylene, and heterocyclylene, either of which rings is optionally substituted). Ar2 = arylene or heteroarylene, each of which is optionally substituted; R5 and R6 = H, alkyl, aryl, and aralkyl; q is 0 or 1; and Ay2 is a 5-6 membered cycloalkyl, heterocyclyl, or heteroaryl substituted with an amino or hydroxy moiety (preferably these groups are ortho to the amide N to which Ay2 is attached) and further optionally substituted; provided that when Cy2 is naphthyl, X1 is -CH2-, Ar2 is Ph, R5 and R6 are H, and q is 0 or 1, Ay2 is not Ph or o-hydroxyphenyl. Although the methods of preparation are not claimed, hundreds of example prepns. are included.

IT **503041-91-6P**, N-(2-Aminophenyl)-3-(4-(((1-(3-benzyl-7-chloro-3,4-dihydro-4-oxoquinazolin-2-yl)ethyl)amino)methyl)phenyl)acrylamide
503044-37-9P, N-(2-Aminophenyl)-4-(((1-(3-benzyl-7-chloro-3,4-dihydro-4-oxoquinazolin-2-yl)propyl)amino)methyl)benzamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of triazinyl and other carboxamides as inhibitors of histone deacetylase for treating cell proliferative disorders)

RN 503041-91-6 CAPLUS
CN 2-Propenamide, N-(2-aminophenyl)-3-[4-[[[1-[7-chloro-3,4-dihydro-4-oxo-3-(phenylmethyl)-2-quinazolinyl]ethyl]amino]methyl]phenyl]- (9CI) (CA INDEX NAME)



RN 503044-37-9 CAPLUS
CN Benzamide, N-(2-aminophenyl)-4-[[[1-[7-chloro-3,4-dihydro-4-oxo-3-(phenylmethyl)-2-quinazolinyl]propyl]amino]methyl]- (9CI) (CA INDEX NAME)



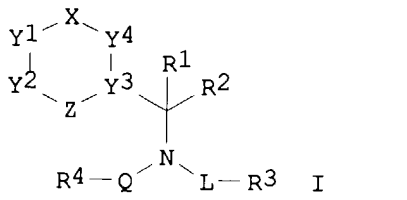
L3 ANSWER 12 OF 30 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:813938 CAPLUS
DOCUMENT NUMBER: 137:337907
TITLE: Preparation of N-(heteroarylalkyl)acylamides as CXCR3 antagonists for treatment of inflammatory or immune conditions
INVENTOR(S): Medina, Julio C.; Johnson, Michael G.; Li, An-Rong; Liu, Jiwen; Huang, Alan Xi; Zhu, Liusheng; Marcus, Andrew P.
PATENT ASSIGNEE(S): Tularik Inc., USA
SOURCE: PCT Int. Appl., 205 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002083143	A1	20021024	WO 2001-US47850	20011211
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2002169159	A1	20021114	US 2001-15532	20011211
EP 1343505	A1	20030917	EP 2001-273533	20011211
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2003069234	A1	20030410	US 2002-164690	20020606
US 2003055054	A1	20030320	US 2002-231895	20020829
NO 2003002612	A	20030805	NO 2003-2612	20030610

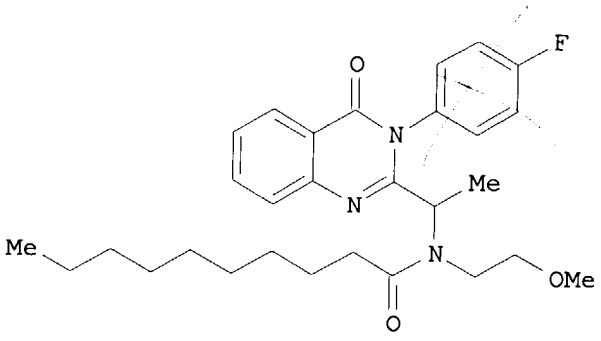
PRIORITY APPLN. INFO.:

US 2000-255241P	P	20001211
US 2001-296499P	P	20010606
US 2001-15532	A1	20011211
WO 2001-US47850	W	20011211

OTHER SOURCE(S): MARPAT 137:337907
GI



I



II

AB Title compds. I [wherein X = a bond, CO, CR5R6, CR5:, SO, SO2, or N: ; Z = a bond, N:, O, S, NR17, or CR7: ; with the proviso that X and Z are not both a bond; L = CO-alkylene or (hetero)alkylene; Q = (hetero)alkylene, CO, OCO, NR8CO, CH2CO, CH2SO, or CH2SO2; or NLQ = heterocyclyl; R1 and R2 = independently H, (hetero)alkyl, or (hetero)aryl; or CR1R2 = (hetero)cyclyl; or CNR2L = heterocyclyl; R3 = OH, alkoxy, NH2, (di)alkylamino, heteroalkyl, heterocyclyl, acylaminoamidino, guanidino, ureido, CN, heteroaryl, carbamoyl, or carboxy; R4 = (hetero)alkyl, (hetero)aryl, etc.; R5 and R6 = independently H, (hetero)alkyl, or (hetero)aryl; or CR5R6 = a ring; R7 and R8 = independently H, (hetero)alkyl, or (hetero)aryl; Y1 and Y2 = independently CR12: N:, O, S, or NR13; Y3 = N or C, wherein C shares a double bond with either Z or Y4; Y4 = NR14, CR14:, N:, NR14CR15R16; R12 = H, halo, OH, NH2, (di)alkylamino, (hetero)alkyl, or (hetero)aryl, with provisos; R13 = H, (hetero)alkyl, (hetero)aryl, etc.; R14 = (hetero)alkyl, (hetero)aryl, etc.; R15 and R16 = independently H or (hetero)alkyl; R17 = H, (hetero)alkyl, (hetero)aryl, etc.; with provisos] were prepared as chemokine receptor modulators, in particular CXCR3 antagonists. For example, anthranilic acid was acylated with propionyl chloride and the amide cyclized using acetic anhydride to give 2-ethylbenzo[d][1,3]oxazine-4-one. Treatment with 4-fluoroaniline, followed by ethylene glycol and NaOH afforded 2-ethyl-3-(4-fluorophenyl)-3H-quinazolin-4-one. Bromination and stepwise addition of 1-amino-2-methoxyethane and decanoyl chloride produced the decanoic acid (quinazolinylethyl)(methoxyethyl)amide II. Approx. one third of the 101 invention compds. tested in a CXCR3 binding assay displayed activity with IC50 values of < 1 μM. I are useful for the treatment of inflammatory and immunoregulatory disorders and diseases, such as multiple sclerosis, rheumatoid arthritis, and type I diabetes (no data).

IT **473718-71-7P**

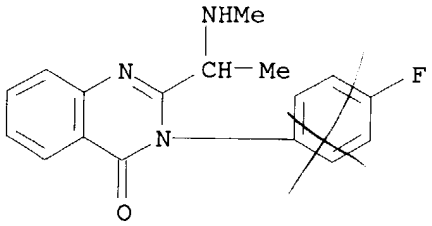
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(CXCR3 antagonist; preparation of N-(heteroarylalkyl)acylamides as CXCR3 antagonists for treatment of inflammatory or immune conditions)

RN 473718-71-7 CAPLUS

CN [1,1'-Biphenyl]-4-acetamide, N-[1-[3-(4-ethoxyphenyl)-3,4-dihydro-4-oxo-2-quinazolinyl]ethyl]- (9CI) (CA INDEX NAME)

(CA INDEX NAME)



L3 ANSWER 17 OF 30 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:167976 CAPLUS
DOCUMENT NUMBER: 134:222723
TITLE: Preparation of quinazolinones for modulating CXR3 function
INVENTOR(S): Schall, Thomas J.; Dairaghi, Daniel J.; McMaster, Brian E.
PATENT ASSIGNEE(S): Chemocentryx, Inc., USA
SOURCE: PCT Int. Appl., 53 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001016114	A2	20010308	WO 2000-US23556	20000825
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1216232	A1	20020626	EP 2000-959489	20000825
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
US 6559160	B1	20030506	US 2000-648329	20000825
US 2003119854	A1	20030626	US 2002-279353	20021023

PRIORITY APPLN. INFO.:

US 1999-151212P	P	19990827
US 2000-648329	A1	20000825
WO 2000-US23556	W	20000825

OTHER SOURCE(S): MARPAT 134:222723
GI

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 13 OF 30 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:935583 CAPLUS
DOCUMENT NUMBER: 136:53759
TITLE: Preparation of N-acylquinazolinonealkylamines as KSP kinesin inhibitors
INVENTOR(S): Finer, Jeffrey T.; Bergnes, Gustav; Feng, Bainian; Smith, Whitney W.; Chabala, John C.; Morgans, David J., Jr.
PATENT ASSIGNEE(S): Cytokinetics, Inc., USA
SOURCE: PCT Int. Appl., 179 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2001098278	A1	20011227	WO 2001-US13901		20010427
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
US 6545004	B1	20030408	US 2000-699047		20001024
JP 2003048881	A2	20030221	JP 2002-156766		20001026
US 6562831	B1	20030513	US 2000-724644		20001128
US 6630479	B1	20031007	US 2000-724713		20001128
EP 1296959	A1	20030402	EP 2001-932769		20010427
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
BR 2001011898	A	20030513	BR 2001-11898		20010427
JP 2004501140	T2	20040115	JP 2002-504234		20010427
ZA 2002010133	A	20030617	ZA 2002-10133		20021213
NO 2002006172	A	20030220	NO 2002-6172		20021220
US 2004023996	A1	20040205	US 2003-312323		20030815
PRIORITY APPLN. INFO.:			US 2000-213104P	P	20000621
			US 2000-699047	A	20001024
			US 1999-198253P	P	19991027
			JP 2001-533122	A3	20001026
			WO 2001-US13901	W	20010427

OTHER SOURCE(S): MARPAT 136:53759
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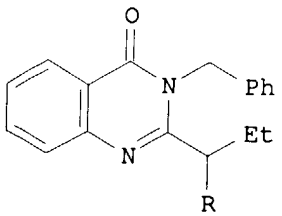


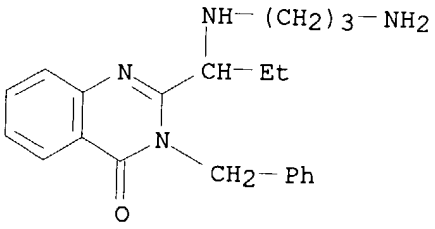
II

not claimed

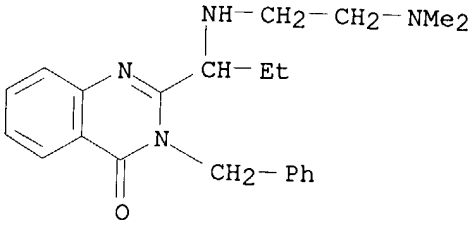
AB R1CR2R2'NRR4 [I; R = H, COR3, SO2R3', CH2R3''; R1 = (un)substituted 3,4-dihydro-4-oxoquinazolin-2-yl; R2,R2' = H, (oxa)alkyl, (hetero)aryl, etc.; R3 = H, alkyl, alkoxy, (hetero)aryl, etc.; R3',R4 = H, alkyl, (hetero)aryl, etc.; R3'' = alkyl, (hetero)aryl, etc.] were prepared Thus, 2-(H2N)C6H4CO2H was amidated by PrCOCl and the cyclized product cyclocondensed with PhCH2NH2 to give, after bromination, quinazolinone II (R = Br) which was converted in 2 steps to II [R = N(COC6H4F-4)CH2CH2NMe2]. Data for biol. activity of I were given.

IT **336119-86-9DP**, resin bound **336119-90-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-acylquinazolinonealkylamines as KSP kinesin inhibitors)

RN 336119-86-9 CAPLUS
CN 4(3H)-Quinazolinone, 2-[1-[(3-aminopropyl)amino]propyl]-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 336119-90-5 CAPLUS
CN 4(3H)-Quinazolinone, 2-[1-[[2-(dimethylamino)ethyl]amino]propyl]-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 14 OF 30 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:387298 CAPLUS
DOCUMENT NUMBER: 135:152997
TITLE: Synthesis of ent-Alantrypinone
AUTHOR(S): Hart, David J.; Magomedov, Nabi A.
CORPORATE SOURCE: Department of Chemistry, The Ohio State University, Columbus, OH, 43210, USA
SOURCE: Journal of the American Chemical Society (2001), 123(25), 5892-5899
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:152997

09/724,897

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

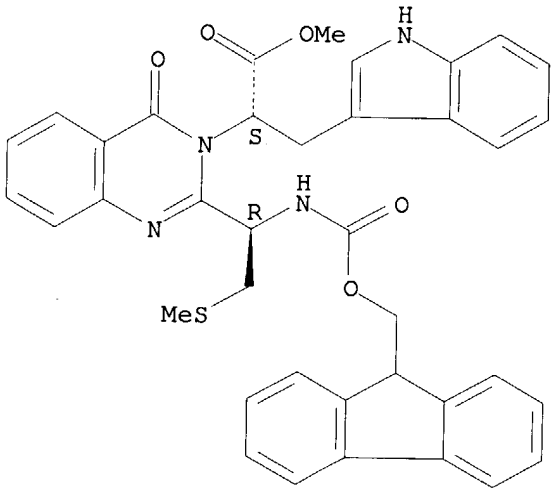
AB This paper presents a synthesis of ent-alantrypinone, the enantiomer of a natural product produced by the fungus Penicillium thymicola. The synthesis revolves around the Li[Me3AlSPh]-promoted isomerization of iminobenzoxazine I to quinazolinone II, an N-acyliminium ion cyclization that converts enamide III to bridged indole, and rearrangement to oxindole title product. Ancillary chemical that involves thermal fragmentation of an iminobenzoxazine to a nitrile ylide and Me2AlSPh-mediated cyclization of oxime ether-ester to pyrrolidinone is also described.

IT **246849-02-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of ent-Alantrypinone)

RN 246849-02-5 CAPLUS

CN 3(4H)-Quinazolineacetic acid, 2-[(1R)-1-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-2-(methylthio)ethyl]-α-(1H-indol-3-ylmethyl)-4-oxo-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 15 OF 30 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:319882 CAPLUS

DOCUMENT NUMBER: 134:326543

TITLE: Methods and compositions utilizing quinazolinones as KSP kinesin modulators

INVENTOR(S): Finer, Jeffrey T.; Bergnes, Gustave; Feng, Bainian; Smith, Whitney W.; Chabala, John C.

PATENT ASSIGNEE(S): Cytokinetics, Inc., USA

SOURCE: PCT Int. Appl., 168 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

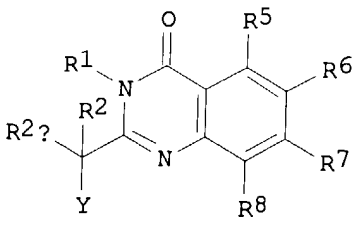
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001030768	A1	20010503	WO 2000-US29585	20001026
WO 2001030768	C2	20020815		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
BR 2000015110	A	20020702	BR 2000-15110	20001026
EP 1226129	A1	20020731	EP 2000-976656	20001026
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003048881	A2	20030221	JP 2002-156766	20001026
JP 2003512461	T2	20030402	JP 2001-533122	20001026
NZ 518480	A	20040227	NZ 2000-518480	20001026
AU 774748	B2	20040708	AU 2001-14398	20001026
US 6562831	B1	20030513	US 2000-724644	20001128
US 6630479	B1	20031007	US 2000-724713	20001128
ZA 2002002930	A	20021028	ZA 2002-2930	20020415
NO 2002001907	A	20020607	NO 2002-1907	20020423
ZA 2002010133	A	20030617	ZA 2002-10133	20021213

PRIORITY APPLN. INFO.:

US 1999-198253P	P	19991027
US 2000-213104P	P	20000621
US 2000-699047	A1	20001024
JP 2001-533122	A3	20001026
WO 2000-US29585	W	20001026

OTHER SOURCE(S): MARPAT 134:326543
GI



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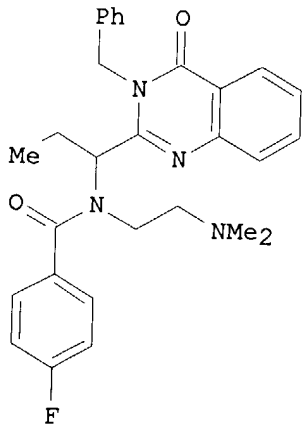


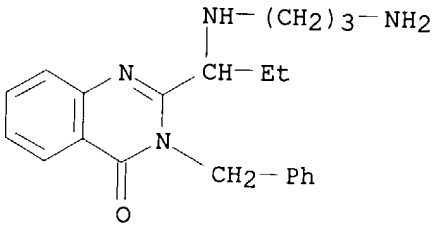
II

AB Quinazolinones (I) [wherein R1 = H, alkyl, (hetero)aryl, or (un)substituted alkyl(hetero)aryl; R2 and R2a = independently H or

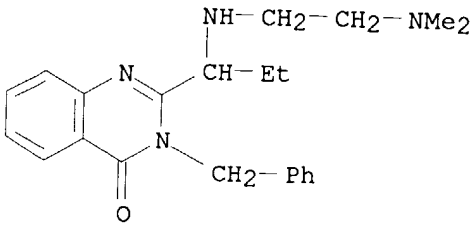
(un)substituted (oxa)alkyl, (hetero)aryl, or alkyl(hetero)aryl; Y = NR4COR3, NR4SO2R3a, NR4CH2R3b, or NHR4; R3 = H, oxaalkyl, or (un)substituted alkyl, (hetero)aryl, alkyl(hetero)aryl, oxaalkylaryl, ether, or amino; R3a = H or (un)substituted alkyl, (hetero)aryl, alkyl(hetero)aryl, or amino; R3b = (un)substituted alkyl, (hetero)aryl, or alkyl(hetero)aryl; R4 = H or (un)substituted alkyl, (hetero)aryl, alkyl(hetero)aryl, or alkylene; R5-R8 = independently H, (fluoro)alkyl, alkoxy, halo, NO2, dialkylamino, alkylsulfonyl, alkylsulfonamido(alkyl or aryl), alkylthio, carboxyalkyl, carboxamido, aminocarbonyl, or (hetero)aryl] were prepared by conventional and solid phase combinatorial synthetic methods as KSP kinesin inhibitors for treatment of cellular proliferative diseases. For example, II was synthesized in a 6-step sequence involving (1) amidation of anthranilic acid with butyryl chloride (65%), (2) cyclization to give 2-propyl-3,1-[4H]benzoxazin-4-one (62%), (3) treatment with PhCH2NH2 to give 2-propyl-3-benzylquinazolin-4-one (67%), bromination (92%), addition of N,N-dimethylethylenediamine (55%), and (6) amidation with p-fluorobenzoyl chloride (65%). I are useful for treating cancer, hyperplasia, restenosis, cardiac hypertrophy, immune disorders, and inflammation (no data). Methods of screening for compds. that will bind to a KSP kinesin or are modulators of KSP kinesin activity are also disclosed.

IT **336119-86-9DP**, resin-bound **336119-90-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of quinazolinone KSP kinesin modulators via conventional and solid phase combinatorial synthetic methods)

RN 336119-86-9 CAPLUS
CN 4(3H)-Quinazolinone, 2-[1-[(3-aminopropyl)amino]propyl]-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 336119-90-5 CAPLUS
CN 4(3H)-Quinazolinone, 2-[1-[[2-(dimethylamino)ethyl]amino]propyl]-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 16 OF 30 CAPLUS

ACCESSION NUMBER: 2001:208250 CAPLUS
DOCUMENT NUMBER: 134:252352
TITLE: Preparation of 3-aryl-2-arylureidoalkylquinazolin-4-ones and related compounds as mediators of hedgehog signaling pathways.
INVENTOR(S): Baxter, Anthony David; Boyd, Edward Andrew; Guichert, Oivin M.; Price, Stephen; Rubin, Lee D.
PATENT ASSIGNEE(S): Curis, Inc., USA
SOURCE: PCT Int. Appl., 177 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001019800	A2	20010322	WO 2000-US25461	20000915
WO 2001019800	A3	20011206		
WO 2001019800	C2	20021003		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1216234	A2	20020626	EP 2000-963551	20000915
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003509414	T2	20030311	JP 2001-523380	20000915
US 6545005	B1	20030408	US 2000-663835	20000915

PRIORITY APPLN. INFO.:

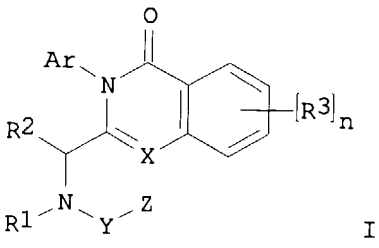
US 1999-154526P	P	19990916
US 1999-159412P	P	19991014
US 1999-162899P	P	19991101
WO 2000-US25461	W	20000915

OTHER SOURCE(S): MARPAT 134:252352

AB R1LX1Y1Z1LX2Y2Z2LR2 [R1, R2 = H, alkyl, (substituted) aryl, aralkyl, heteroaryl, heteroarylalkyl; L = null, alkyl, alkenyl, alkynyl, (CH2)nO(CH2)p, etc.; n, p = 0-10; X1, X2 = NR8, O, S, Se, N:N, ON:CH, heterocyclyl, bond, etc.; Y1, Y2 = CO, CS, SO2, SO, C(:NCN), heteroaryl, bond, etc.; Z1, Z2 = NR8, O, S, Se, N:N, ON:CH, heterocyclyl, bond, etc.; R8 = H, alkyl, (substituted) aryl, aralkyl, heteroaryl, heteroaralkyl, etc.], were prepared Thus, triphosgene in EtOAc was added to 4-nitro-3-trifluoromethylaniline in EtOAc followed by stirring and reflux. The mixture was concentrated, dissolved in CHCl3, and treated with 3-(4-fluorophenyl)-2-(1-methylaminoethyl)-4-oxo-3,4-dihydroquinazoline in CHCl3 to give 97% 1-[1-[3-(4-fluorophenyl)-4-oxo-3,4-dihydroquinazolin-2-yl]ethyl]-3-(3-trifluoromethyl-4-nitrophenyl)-1-methylurea. The latter inhibited sonic hedgehog-induced Gli transcription activity with IC50 <5 μM.

IT **330796-26-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 3-aryl-2-arylureidoalkylquinazolin-4-ones and related compds. as mediators of hedgehog signaling pathways)

RN 330796-26-4 CAPLUS
CN 4(3H)-Quinazolinone, 3-(4-fluorophenyl)-2-[1-(methylamino)ethyl]- (9CI)



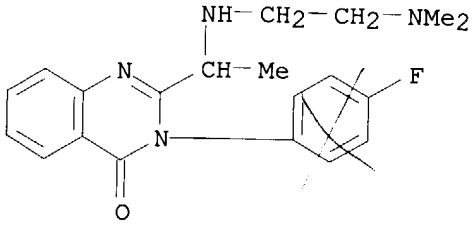
I

AB The title compds. [I; n = 0-4; Ar = (un)substituted aryl, heteroaryl; R1 = (un)substituted C5-15 alkyl; R2 = (un)substituted C1-8 alkyl; X = CH, N; Y = (un)substituted alkylene, heteroalkylene; Z = NR4R5 (R4, R5 = H, alkyl; NR4R5 = 5-7 membered ring)] that bind to the CXCR3 chemokine receptor and which are useful for treating diseases associated with CXCR3 activity, such as multiple sclerosis, were prepared E.g., a multi-step synthesis of the quinazolinone I [Ar = 4-C6H4; R1 = decanoyl; R2 = Me; Y = (CH2)2; Z = NMe2; R3 = H] which showed IC50 of ≤ 0.8 μM against CXCR3 chemokine receptor binding, was given.

IT **329190-50-3P 329190-54-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of quinazolinones for modulating CXR3 function)

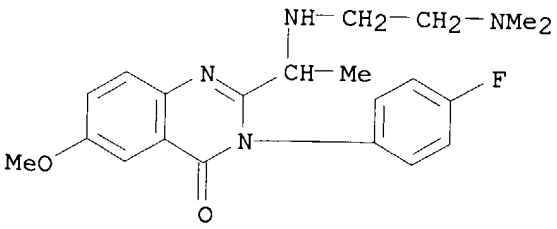
RN 329190-50-3 CAPLUS

CN 4(3H)-Quinazolinone, 2-[1-[[2-(dimethylamino)ethyl]amino]ethyl]-3-(4-fluorophenyl)- (9CI) (CA INDEX NAME)



RN 329190-54-7 CAPLUS

CN 4(3H)-Quinazolinone, 2-[1-[[2-(dimethylamino)ethyl]amino]ethyl]-3-(4-fluorophenyl)-6-methoxy- (9CI) (CA INDEX NAME)



L3 ANSWER 18 OF 30 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:91539 CAPLUS

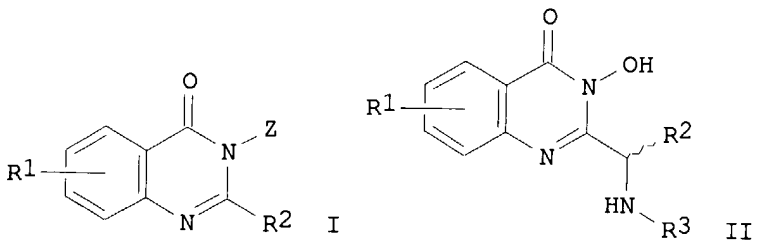
DOCUMENT NUMBER: 134:147610

TITLE: Compositions containing N-amino- and N-hydroxy-quinazolinones and methods for preparing

combinatorial libraries thereof
INVENTOR(S): Gao, Yun
PATENT ASSIGNEE(S): Sepracor Inc., USA
SOURCE: U.S., 15 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6184377	B1	20010206	US 1997-990855	19971215
US 2001018518	A1	20010830	US 2001-775339	20010201
US 6429311	B2	20020806		

PRIORITY APPLN. INFO.: US 1997-990855 A1 19971215
OTHER SOURCE(S): MARPAT 134:147610
GI



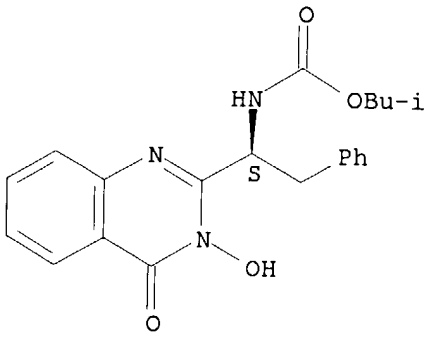
AB The invention is directed to certain N-amino- and N-hydroxy-quinazolinone compds., and methods for their synthesis. The compds. may find use in combinatorial libraries. More specifically, the invention is directed to the synthesis of 3-hydroxy- and 3-amino-4(1H)-quinazolinones via the reaction of an appropriate 2-aminobenzamide compound with a carboxylic acid or acyl halide at ambient temperature, performed on a solid support or in solution

In particular, the compds. are prepared via supported compds. I [R1 = H, halo, alkyl, OH, alkoxy, etc.; or adjacent (R1)2 = (hetero)aromatic fusion; R2 = (un)substituted alkyl, alkoxy, N-protected amino acid residue, Ph, etc.; Z = NHCO2CH2-Sup, OCH2-Sup, etc.; Sup = solid support]. For instance, Sup-ONH2 reacted with 15 isatoic anhydrides to give 15 supported 2-amino-N-hydroxybenzamides Sup-ONH-CO-C6H4-n(R1)n-NH2-2. The latter compds. were mixed into 5 groups of 3, and each group was then split 16 ways and cyclized sep. with each of 16 Fmoc-protected amino acids, using PyBrOP in DMAC as the condensing agent. Each of the 80 resultant Fmoc-protected quinazolinone mixts. was deprotected with piperidine, separated into 24 wells of a reactor block, and reacted with a selection of 8 chloroformates, 8 sulfonyl chlorides, and 8 isocyanates. The resulting 1920 product mixts. were treated with TFA to cleave the resin, yielding a library of 5760 different 3-hydroxyquinazolin-4-ones [II; R1 = H, Me, MeO, halo, and/or NO2; R2 = amino acid sidechain; R3 = other sidechain forming a carbamate, sulfonamide, or urea group], as 3-compound mixts., which were stored for future bioassay.

IT **324528-54-3P 324528-55-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(target compound; methods for preparation of N-amino- and N-hydroxy-quinazolinones and combinatorial libraries thereof)
RN 324528-54-3 CAPLUS

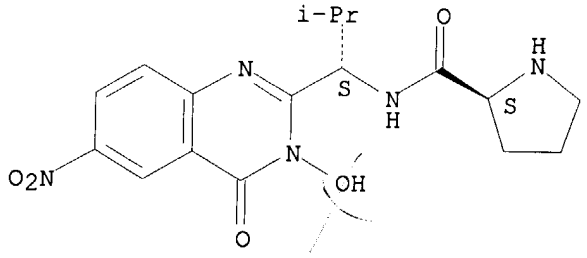
CN Carbamic acid, [(1S)-1-(3,4-dihydro-3-hydroxy-4-oxo-2-quinazolinyl)-2-phenylethyl]-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 324528-55-4 CAPLUS
CN 2-Pyrrolidinecarboxamide, N-[(1S)-1-(3,4-dihydro-3-hydroxy-6-nitro-4-oxo-2-quinazolinyl)-2-methylpropyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



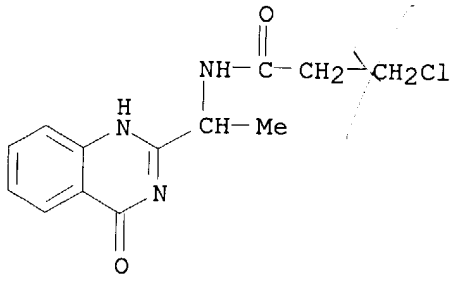
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 19 OF 30 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:752919 CAPLUS
DOCUMENT NUMBER: 133:355320
TITLE: Optical resolution of a series of potential cholecystokinin antagonist 4(3H)-quinazolone derivatives by chiral liquid chromatography on α1-acid glycoprotein stationary phase
AUTHOR(S): Gyimesi-Forras, Krisztina; Szasz, Gyorgy; Gergely, Andras; Szabo, Monika; Kokosi, Jozsef
CORPORATE SOURCE: Institute of Pharmaceutical Chemistry, Semmelweis University, Budapest, H-1092, Hung.
SOURCE: Journal of Chromatographic Science (2000), 38(10), 430-434
CODEN: JCHSBZ; ISSN: 0021-9665
PUBLISHER: Preston Publications
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Optical resolution of the enantiomers of new 4(3H)-quinazolone derivs. was investigated using the α1-acid glycoprotein chiral stationary phase (Chiral-AGP). Stereoselective separation of the model compds. can be controlled by varying the pH and adding uncharged organic modifiers

(acetonitrile and 2-propanol) to the mobile phase. For the majority of quinazolone derivs., Chiral-AGP is proved to be an excellent enantioselector, because optimized chromatog. conditions allow for the baseline separation of the enantiomers. Separation factors between 1.19 and 1.85 are obtained. The effects of acetonitrile and 2-propanol on the chromatog. behavior of the model compds. are quite different because of their different hydrophobic- and hydrogen-bonding properties. The eluent pH and organic modifier concentration also contributes to the chiral recognition by altering the protein environment. The anal. of the exptl. results leads to new information about the chromatog. mechanism on a Chiral-AGP surface. (c) 2000 Preston Publications.

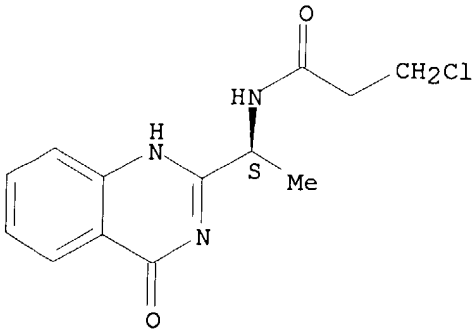
IT **172420-43-8 304866-32-8 304866-33-9**
RL: ANT (Analyte); ANST (Analytical study)
(optical resolution of potential cholecystokinin antagonist 4(3H)-quinazolone derivs. by chiral liquid chromatog. on α1-acid glycoprotein stationary phase)

RN 172420-43-8 CAPLUS
CN Propanamide, 3-chloro-N-[1-(1,4-dihydro-4-oxo-2-quinazolinyl)ethyl]- (9CI) (CA INDEX NAME)



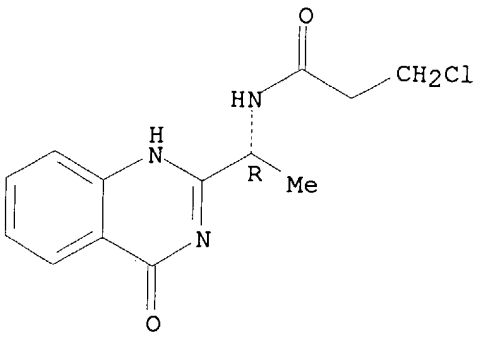
RN 304866-32-8 CAPLUS
CN Propanamide, 3-chloro-N-[(1S)-1-(1,4-dihydro-4-oxo-2-quinazolinyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 304866-33-9 CAPLUS
CN Propanamide, 3-chloro-N-[(1R)-1-(1,4-dihydro-4-oxo-2-quinazolinyl)ethyl]- (9CI) (CA INDEX NAME)

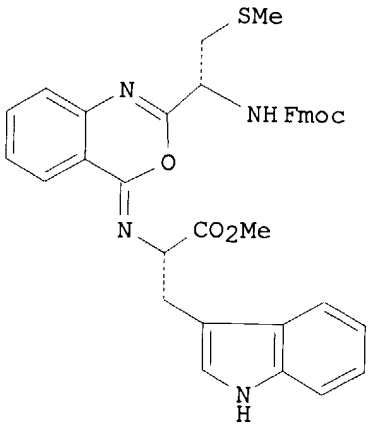
Absolute stereochemistry.



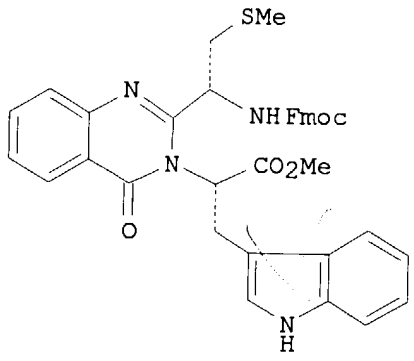
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 20 OF 30 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:461992 CAPLUS
DOCUMENT NUMBER: 131:286686
TITLE: Synthesis of (-)-alantrypinone
AUTHOR(S): Hart, David J.; Magomedov, Nabi
CORPORATE SOURCE: Department of Chemistry, The Ohio State University, Columbus, OH, 43210, USA
SOURCE: Tetrahedron Letters (1999), 40(30), 5429-5432
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 131:286686
GI



I



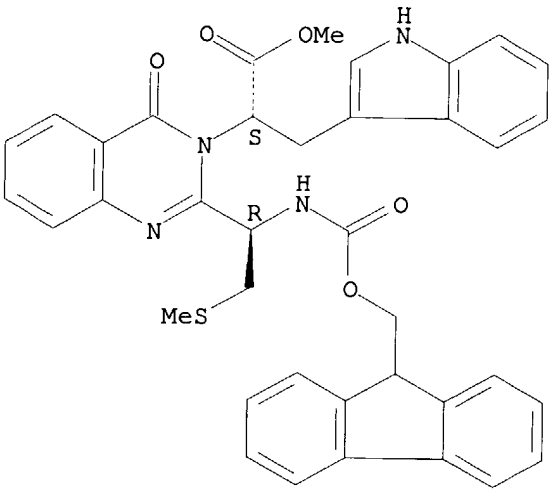
II

AB A synthesis of (-)-alantrypinone is described. The synthesis features the use of [Me3AlSPh]Li as a promoter of a 4-iminobenzoxazine I to 4-quinazolinone II rearrangement and as a reagent for the deprotection of an Fmoc-protected amino acid derivative

IT **246849-02-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of (-)-alantrypinone)

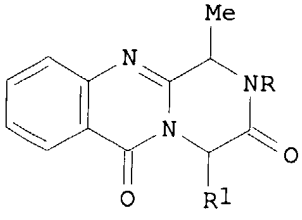
RN 246849-02-5 CAPLUS
CN 3(4H)-Quinazolineacetic acid, 2-[(1R)-1-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-2-(methylthio)ethyl]-α-(1H-indol-3-ylmethyl)-4-oxo-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 21 OF 30 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:663413 CAPLUS
DOCUMENT NUMBER: 130:38348
TITLE: Nitrogen bridgehead compounds. Part 90. An efficient versatile synthesis of 1-methyl-2-substituted 1,2,3,4-tetrahydro-6H-pyrazino[2,1-b]quinazoline-3,6-diones
AUTHOR(S): Kokosi, Jozsef; Almasi, Janos; Podanyi, Benjamin; Feher, Miklos; Bocskei, Zsolt; Simon, Kalman; Hermecz, Istvan
CORPORATE SOURCE: Institute for Pharmaceutical Chemistry Semmelweis University of Medicine, Budapest, 1092, Hung.
SOURCE: Heterocycles (1998), 48(9), 1851-1866
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:38348
GI



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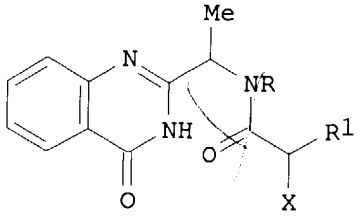
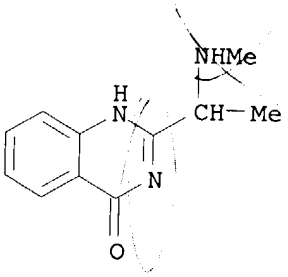


II

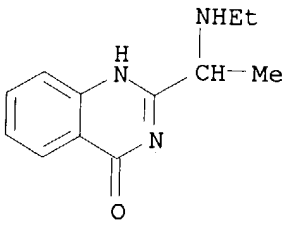
AB A versatile synthesis of 2-substituted 1-methyl- and 1,4-dimethyl-1,2,3,4-tetrahydro-6H-pyrazino[2,1-b]quinazoline-3,6-diones I (R = H, Et, Ph, etc., R1 = H, Me) is presented, starting from 2-(1-bromoethyl)quinazolin-4(3H)-one. The key step of the reaction sequence is the diastereoselective cyclization of 2-{[1-(N-2-haloacyl)-N-substituted amino]ethyl}quinazolin-4(3H)-ones II (R1 = H, X = Cl; R1 = Me, X = Br). Usually 1,4-di-Me derivs. are obtained as pure racemic cis-compds. (2-alkyl and 2-benzyl derivs.), or a mixture of diastereomers, containing the 4-Me group in quasi-axial position.

IT **143993-15-1P 143993-16-2P 143993-17-3P**
143993-18-4P 143993-20-8P 216596-07-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of methylpyrazinoquinazolinediones)

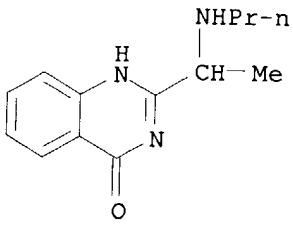
RN 143993-15-1 CAPLUS
CN 4(1H)-Quinazolinone, 2-[1-(methylamino)ethyl]- (9CI) (CA INDEX NAME)



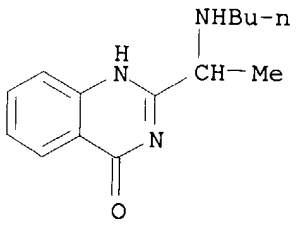
RN 143993-16-2 CAPLUS
CN 4(1H)-Quinazolinone, 2-[1-(ethylamino)ethyl]- (9CI) (CA INDEX NAME)



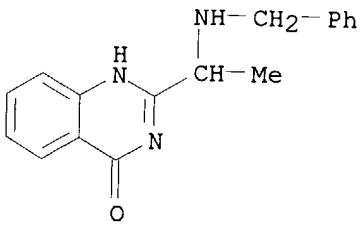
RN 143993-17-3 CAPLUS
CN 4(1H)-Quinazolinone, 2-[1-(propylamino)ethyl]- (9CI) (CA INDEX NAME)



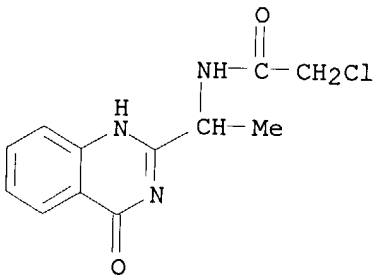
RN 143993-18-4 CAPLUS
CN 4(1H)-Quinazolinone, 2-[1-(butylamino)ethyl]- (9CI) (CA INDEX NAME)



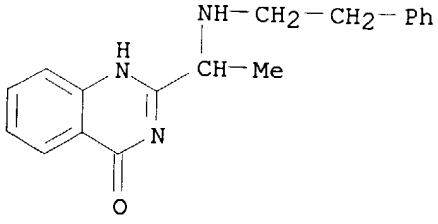
RN 143993-20-8 CAPLUS
CN 4(1H)-Quinazolinone, 2-[1-[(phenylmethyl)amino]ethyl]- (9CI) (CA INDEX NAME)



RN 216596-07-5 CAPLUS
CN Acetamide, 2-chloro-N-[1-(1,4-dihydro-4-oxo-2-quinazolinyl)ethyl]- (9CI) (CA INDEX NAME)



IT **143993-21-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of methylpyrazinoquinazolinediones)
RN 143993-21-9 CAPLUS
CN 4(1H)-Quinazolinone, 2-[1-[(2-phenylethyl)amino]ethyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 22 OF 30 CAPLUS COPYRIGHT 2004 ACS on STN

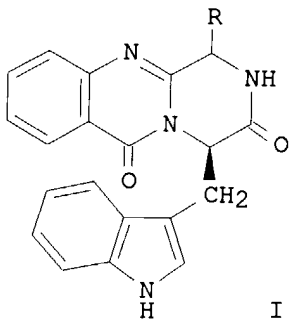
ACCESSION NUMBER: 1998:229741 CAPLUS
DOCUMENT NUMBER: 128:257597

TITLE: Total Synthesis of the Quinazoline Alkaloids (-)-Fumiquinazoline G and (-)-Fiscalin B

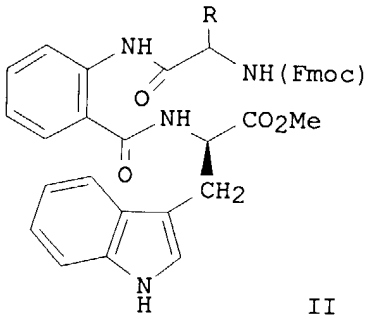
AUTHOR(S): Wang, Haishan; Ganesan, A.
CORPORATE SOURCE: Institute of Molecular and Cell Biology, National University of Singapore, Singapore, 117609, Singapore

SOURCE: Journal of Organic Chemistry (1998), 63(8), 2432-2433
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 128:257597

GI



I



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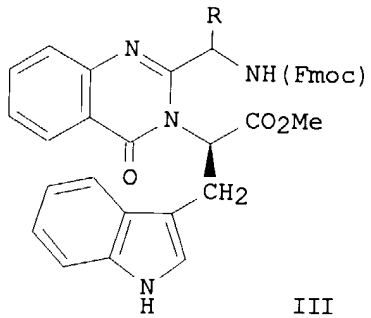


III

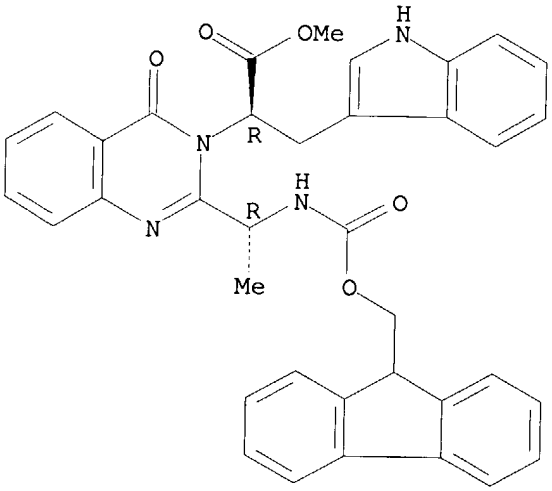
AB (-)-Fumiquinazoline G (I; R = β-Me) and (-)-fiscalin B (I; R = α-CHMe2) were synthesized in four and five steps resp. from D-tryptophan Me ester. The key transformation involved dehydrative cyclization of linear tripeptides II (Fmoc = 9-fluorenylmethoxycarbonyl, R = β-Me, α-CHMe2, resp.) to quinazolin-4-ones III. The methodol. is also applicable to the synthesis of quinazolinones with sterically bulky 2,3-substitution.

IT **205042-96-2P 205042-98-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(total synthesis of the quinazoline alkaloids fumiquinazoline G and fiscalin B from D-tryptophan Me ester)

RN 205042-96-2 CAPLUS

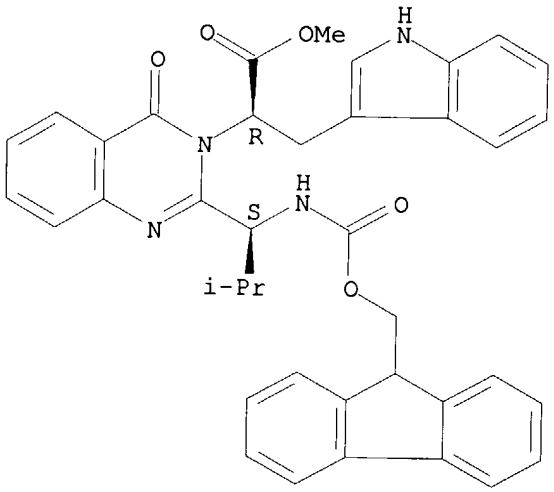
CN 3(4H)-Quinazolineacetic acid, 2-[1-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]ethyl]-α-(1H-indol-3-ylmethyl)-4-oxo-, methyl ester, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 205042-98-4 CAPLUS
CN 3(4H)-Quinazolineacetic acid, 2-[1-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-2-methylpropyl]-α-(1H-indol-3-ylmethyl)-4-oxo-, methyl ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 23 OF 30 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:39965 CAPLUS
DOCUMENT NUMBER: 128:102060
TITLE: Synthesis heterocondensed 4(3H)-quinazolinones: 1,2,4-triazino[6,1-b]- and 1,2,5-triazepino[2,3-b]quinazolinones

09/724,897

AUTHOR(S): Kiss, Arpad; Almasi, Janos; Szabo, Monika; Kokosi, Jozsef; Hermecz, Istvan

CORPORATE SOURCE: Semmelweis Orvostudomanyi Egyetem, Gyogyszereszi Kemiai Intezet, Budapest, H-1092, Hung.

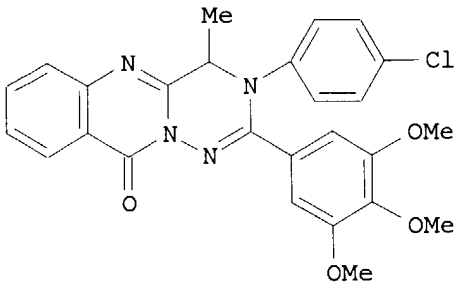
SOURCE: Acta Pharmaceutica Hungarica (1997), 67(6), 255-261
CODEN: APHGAO; ISSN: 0001-6659

PUBLISHER: Magyar Gyogyszereszeti Tarsasag

DOCUMENT TYPE: Journal

LANGUAGE: Hungarian

GI



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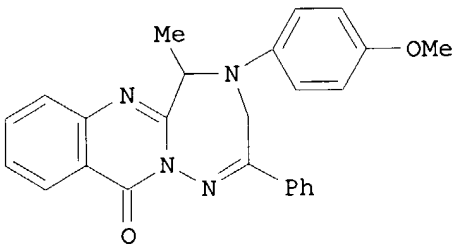


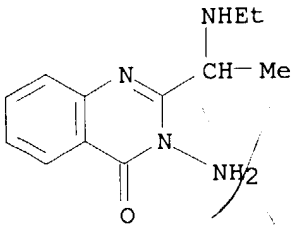
II

AB Title compds. such as I and II were prepared from 2-alkyl-3,1-benzoxazinones via 2-[(alkylamino)alkyl]-3-amino-4(3H)-quinazolinones.

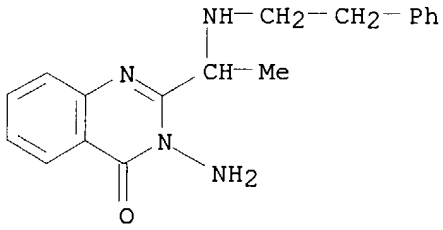
IT **201418-53-3P 201418-54-4P 201418-55-5P 201418-56-6P 201418-62-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1,2,4-triazino[6,1-b]- and 1,2,5-triazepino[2,3-b]quinazolinones)

RN 201418-53-3 CAPLUS

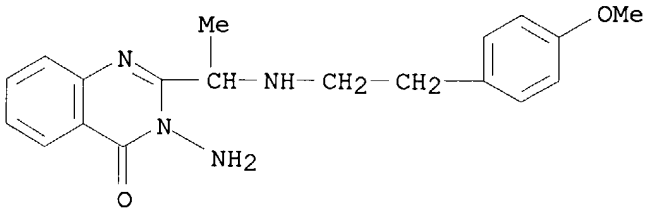
CN 4(3H)-Quinazolinone, 3-amino-2-[1-(ethylamino)ethyl]- (9CI) (CA INDEX NAME)



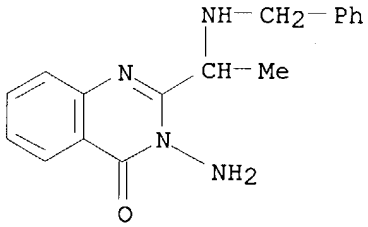
RN 201418-54-4 CAPLUS
CN 4(3H)-Quinazolinone, 3-amino-2-[1-[(2-phenylethyl)amino]ethyl]- (9CI) (CA INDEX NAME)



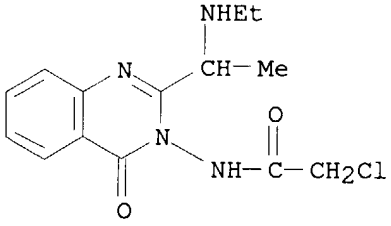
RN 201418-55-5 CAPLUS
CN 4(3H)-Quinazolinone, 3-amino-2-[1-[[2-(4-methoxyphenyl)ethyl]amino]ethyl]- (9CI) (CA INDEX NAME)



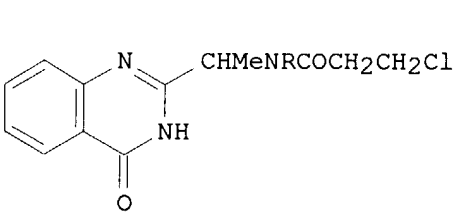
RN 201418-56-6 CAPLUS
CN 4(3H)-Quinazolinone, 3-amino-2-[1-[(phenylmethyl)amino]ethyl]- (9CI) (CA INDEX NAME)



RN 201418-62-4 CAPLUS
CN Acetamide, 2-chloro-N-[2-[1-(ethylamino)ethyl]-4-oxo-3(4H)-quinazolinyl]- (9CI) (CA INDEX NAME)



L3 ANSWER 24 OF 30 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:557328 CAPLUS
DOCUMENT NUMBER: 125:328537
TITLE: Synthesis and cyclization of new quinazolone derivatives to [1,4]oxazepino- and [1,4]diazepino[3,4-b]quinazolones
AUTHOR(S): Szabo, Monika; Orfi, Laszlo; Kokosi, Jozsef; Hermecz, Istvan; Kovacs, Attila
CORPORATE SOURCE: Semmelweis Orvostudomanyi Egyetem, Gyogyszereszi Kemiai Intezet, Budapest, 1092, Hung.
SOURCE: Magyar Kemiai Folyoirat (1996), 102(8), 343-355
CODEN: MGKFA3; ISSN: 0025-0155
PUBLISHER: Magyar Kemikusok Egyesulete
DOCUMENT TYPE: Journal
LANGUAGE: Hungarian
GI



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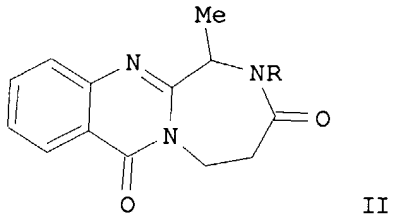
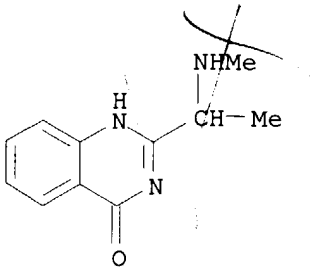


II

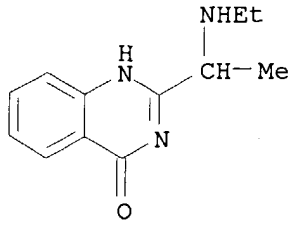
AB Original routes have been developed for the synthesis of new heterocondensed quinazolones: [1,4]oxazepino[3,4-b]quinazolone and [1,4]diazepino[3,4-b]quinazolones. E.g., cyclization of quinazolone I (R = 4-MeOC6H4) gave [1,4]diazepino[3,4-b]quinazolone II.

IT **143993-15-1 143993-16-2 143993-17-3 143993-18-4 143993-20-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of quinazolones, [1,4]oxazepino-, and [1,4]diazepino[3,4-b]quinazolones)

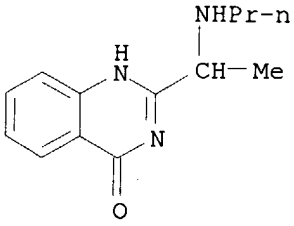
RN 143993-15-1 CAPLUS
CN 4(1H)-Quinazolinone, 2-[1-(methylamino)ethyl]- (9CI) (CA INDEX NAME)



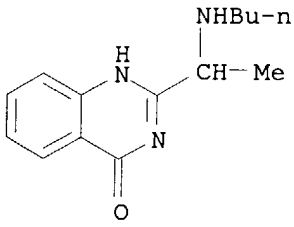
RN 143993-16-2 CAPLUS
CN 4(1H)-Quinazolinone, 2-[1-(ethylamino)ethyl]- (9CI) (CA INDEX NAME)



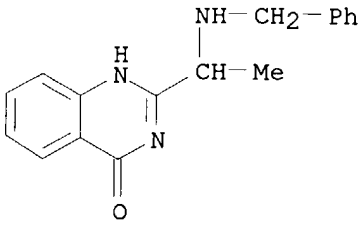
RN 143993-17-3 CAPLUS
CN 4(1H)-Quinazolinone, 2-[1-(propylamino)ethyl]- (9CI) (CA INDEX NAME)



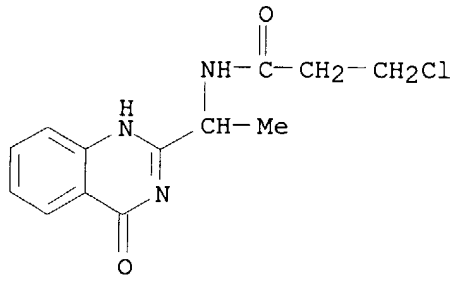
RN 143993-18-4 CAPLUS
CN 4(1H)-Quinazolinone, 2-[1-(butylamino)ethyl]- (9CI) (CA INDEX NAME)



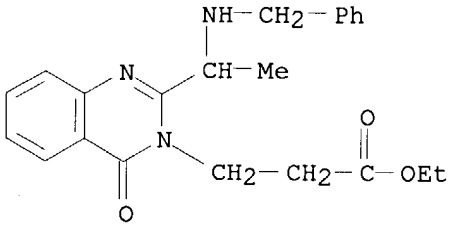
RN 143993-20-8 CAPLUS
CN 4(1H)-Quinazolinone, 2-[1-[(phenylmethyl)amino]ethyl]- (9CI) (CA INDEX NAME)



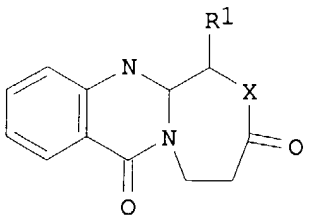
IT **172420-43-8P 173914-73-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of quinazolones, [1,4]oxazepino-, and [1,4]diazepino[3,4-b]quinazolones)
RN 172420-43-8 CAPLUS
CN Propanamide, 3-chloro-N-[1-(1,4-dihydro-4-oxo-2-quinazolinyl)ethyl]- (9CI) (CA INDEX NAME)



RN 173914-73-3 CAPLUS
CN 3(4H)-Quinazolinepropanoic acid, 4-oxo-2-[1-[(phenylmethyl)amino]ethyl]-, ethyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 25 OF 30 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:991676 CAPLUS
DOCUMENT NUMBER: 124:176002
TITLE: Synthesis of potential CCK antagonist quinazolone derivatives
AUTHOR(S): Szabo, Monika; Kokosi, Jozsef; Kovacs, Attila; Orfi, Laszlo
CORPORATE SOURCE: Gyogyszereszi kemiai Intezet, Semmelweis Orvostudomanyi Egyetem, Budapest, Hung.
SOURCE: Acta Pharmaceutica Hungarica (1995), 65(5), 175-81
CODEN: APHGAO; ISSN: 0001-6659
PUBLISHER: Ifjusagi Lap- es Konyvkiado Vallalat
DOCUMENT TYPE: Journal
LANGUAGE: Hungarian
GI



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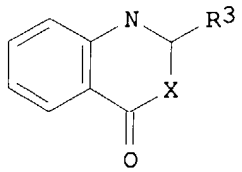


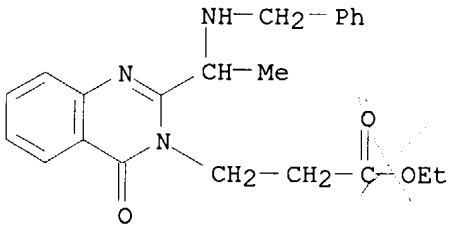
II

AB An alternative route has been developed for the synthesis of [1,4]diazepino[3,4-b]quinazolones (I; X = NR2, R1 = H, R2 = Et, Ph,

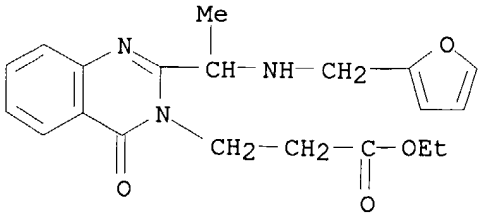
4-MeC6H4, 4-MeOC6H4, 4-EtOC6H4, 4-ClC6H4, 4-BrC6H4, 4-AcC6H4, 4-Me2NC6H4; R1 = Me, R2 = Me, Et, Pr, CHMe2, Bu, Me2CHCH2,CH2CH2NMe2, CH2Ph, Ph, 4-MeC6H4, 4-MeOC6H4, 4-EtOC6H4, 4-ClC6H4, 4-BrC6H4), a new ring system of heterocondensed quinazolones. 2,3-Bifunctional quinazolones II (X = NCH2CH2CO2H, R3 = Me, Et) were synthesized by halogenation of 2-alkylbenzoazones II (X = O, R3 = Me, Et) with β-alanine. The reaction of haloalkyl compds. II (X = NCH2CH2CO2H, R3 = CH2Br, CHBrMe, CHBr2) with N-nucleophiles produces [1,4]oxazepino-[3,4-b]quinazolones I (X = O, R1 = Me), a new heterocyclic ring system, and 3-[2'-hydroxyethyl-, or 2'-chloroethyl-4'-oxo(3'H)-quinazoline-3'-yl]propionamides II (R3 = CHBr2, CHMeOH, X = NCH2CH2CONHR2) in consecutive reaction. The cyclization of 2-aminoalkyl-3-propionates II (X = CH2CH2CO2Et, R3 = CHMeNHR2) resulted in the title compds. I (R1 = Me, X = NC6H4OMe-4). Phys. data and properties of the newly synthesized compds. such as IR, UV and NMR spectra were obtained for all compds. reported.

IT **173914-73-3P 173914-74-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(alternative synthesis of diazepinoquinazolones as potential CCK antagonists)

RN 173914-73-3 CAPLUS
CN 3(4H)-Quinazolinepropanoic acid, 4-oxo-2-[1-[(phenylmethyl)amino]ethyl]-, ethyl ester (9CI) (CA INDEX NAME)



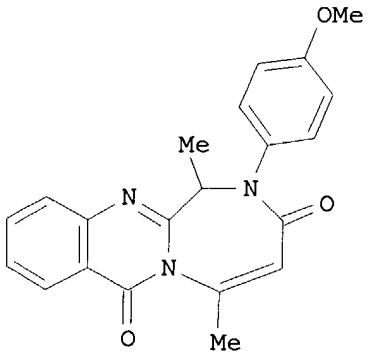
RN 173914-74-4 CAPLUS
CN 3(4H)-Quinazolinepropanoic acid, 2-[1-[(2-furanylmethyl)amino]ethyl]-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 26 OF 30 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:	1995:855051 CAPLUS
DOCUMENT NUMBER:	124:86929
TITLE:	Synthesis of potential CCK antagonist quinazolone derivatives
AUTHOR(S):	Szabo, Monika; Kokosi, Jozsef; Orfi, Laszlo
CORPORATE SOURCE:	Gyogyszereszi Kemiai Intezet, Semmelweis Orvostudomanyi Egyetem, Budapest, Hung.
SOURCE:	Acta Pharmaceutica Hungarica (1995), 65(4), 133-8 CODEN: APHGAO; ISSN: 0001-6659

PUBLISHER: Ifjusagi Lap- es Konyvkiado Vallalat
DOCUMENT TYPE: Journal
LANGUAGE: Hungarian
GI

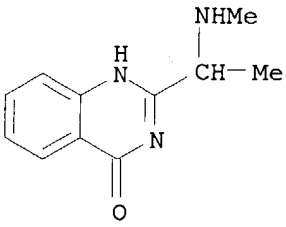


I

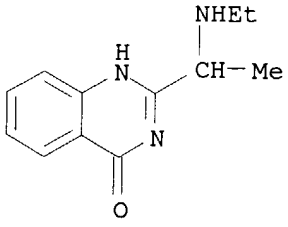
AB An original route has been found for the synthesis of [1,4]diazepinoquinazolones (e.g., I), a new ring system of heterocondensed quinazolones. These anthranilic acid-alanine-β-alanine cyclopeptide derivs. constitute a structural moiety of asperlicin, the first natural cholecystokinin antagonist alkaloid. These compds. are therefore potential CCK antagonists. The new compds. were prepared via condensation of 2-(aminoalkyl)quinazolones, obtained from 2-alkylquinazolones by side-chain substitution, with 1,3-bifunctional reagents. We studied the cyclization process under basic, acidic and phase-transfer catalyzed conditions. The structures of the synthesized compds. were characterized by IR, UR and NMR spectroscopy.

IT **143993-15-1 143993-16-2 143993-17-3**
143993-18-4 143993-20-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of [1,4]diazepinoquinazolones as potential CCK antagonists)

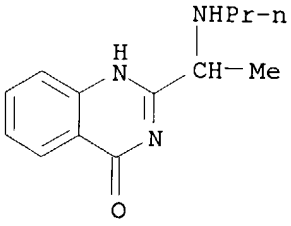
RN 143993-15-1 CAPLUS
CN 4(1H)-Quinazolinone, 2-[1-(methylamino)ethyl]- (9CI) (CA INDEX NAME)



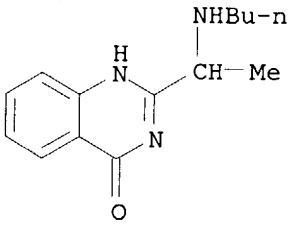
RN 143993-16-2 CAPLUS
CN 4(1H)-Quinazolinone, 2-[1-(ethylamino)ethyl]- (9CI) (CA INDEX NAME)



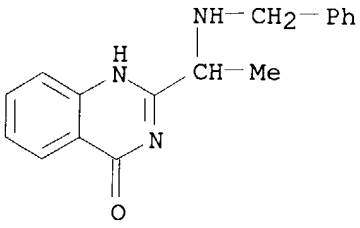
RN 143993-17-3 CAPLUS
CN 4(1H)-Quinazolinone, 2-[1-(propylamino)ethyl]- (9CI) (CA INDEX NAME)



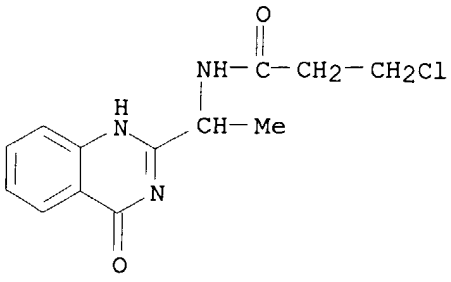
RN 143993-18-4 CAPLUS
CN 4(1H)-Quinazolinone, 2-[1-(butylamino)ethyl]- (9CI) (CA INDEX NAME)



RN 143993-20-8 CAPLUS
CN 4(1H)-Quinazolinone, 2-[1-[(phenylmethyl)amino]ethyl]- (9CI) (CA INDEX NAME)



IT **172420-43-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of [1,4]diazepinoquinazolones as potential CCK antagonists)
RN 172420-43-8 CAPLUS
CN Propanamide, 3-chloro-N-[1-(1,4-dihydro-4-oxo-2-quinazolinyl)ethyl]- (9CI) (CA INDEX NAME)



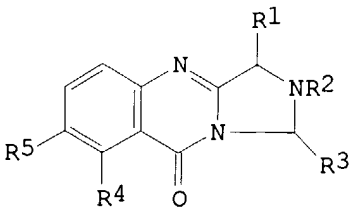
L3 ANSWER 27 OF 30 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:	1992:612519 CAPLUS
DOCUMENT NUMBER:	117:212519
TITLE:	Process for producing imidazo[5,1-b]quinazolin-9-one derivatives and pharmaceutically acceptable salts thereof, as well as pharmaceutical compositions comprising such as active ingredient
INVENTOR(S):	Kokosi, Jozsef; Orfi, Laszlo; Szasz, Gyorgy; Hermecz, Istvan; Kapui, Zoltan; Szabo, Monika
PATENT ASSIGNEE(S):	Semmelweis Orvostudomanyi Egyetem, Hung.
SOURCE:	Hung. Teljes, 21 pp. CODEN: HUXXBU
DOCUMENT TYPE:	Patent
LANGUAGE:	Hungarian
FAMILY ACC. NUM. COUNT:	1
PATENT INFORMATION:	

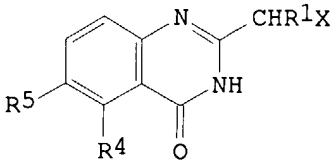
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
HU 59411	A2	19920528	HU 1990-4983	19900810
PRIORITY APPLN. INFO.:			HU 1990-4983	19900810

OTHER SOURCE(S): CASREACT 117:212519; MARPAT 117:212519

GI



I



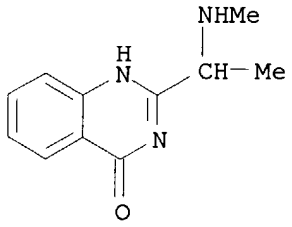
II

AB Thrombocyte aggregation inhibiting racemic or optically active imidazoquinazolinones I [R1 = H, alkyl, aryl, aralkyl; R2 = H, alkyl, aryl, aralkyl, aminoalkyl; R3 = H, alkyl, aryl, aralkyl; R4, R5 = (equivalently or variably) halo, Me, OMe] were prepared by sequential amination of II (X = halo) with R2NH2 in the presence of catalytic I2 or inorg. iodide and cyclization of resulting II (X = NHR2) with aldehyde R3CHO. Thus, bromination of 1.7 g 2-ethylquinazolin-4-one in 20 mL HOAc with a 10 mL glacial HOAc solution of 1.6 g Br2 in the presence of 0.82 g anhydrous NaOAc afforded 78.6% II (X = Br, R1 = Me, R4 = R5 = H); amination of 0.01 mol of the latter with 0.04 mol EtNH2 in the presence of 0.001 mol

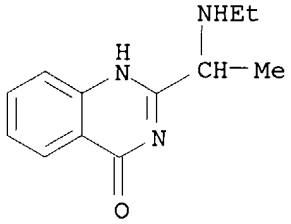
KI in 10 mL H2O afforded 69% of the corresponding II (X = NHEt); finally, 0.01 mol of the latter aminoalkyl derivative was cyclized with 0.30 g paraformaldehyde in 30 mL alc. in the presence of 0.001 mol Et3N, affording 55% I (R1= Me, R2 = Et, R3 = H, R4 = R5 = H). The thrombocyte aggregation inhibiting capacity of I (R1= Me, R2 = Et, R3 = H, R4 = R5 = H) as well as other I derivs. was examined

IT **143993-15-1P 143993-16-2P 143993-17-3P**
143993-18-4P 143993-19-5P 143993-20-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of, with aldehyde)

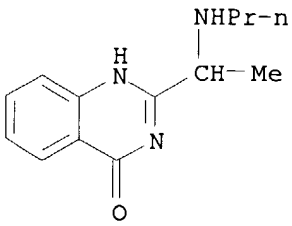
RN 143993-15-1 CAPLUS
CN 4(1H)-Quinazolinone, 2-[1-(methylamino)ethyl]- (9CI) (CA INDEX NAME)



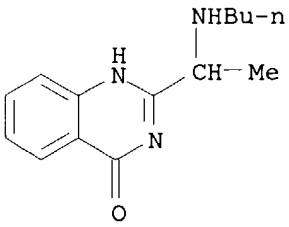
RN 143993-16-2 CAPLUS
CN 4(1H)-Quinazolinone, 2-[1-(ethylamino)ethyl]- (9CI) (CA INDEX NAME)



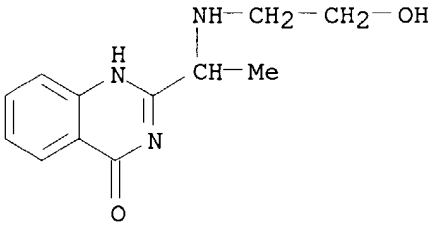
RN 143993-17-3 CAPLUS
CN 4(1H)-Quinazolinone, 2-[1-(propylamino)ethyl]- (9CI) (CA INDEX NAME)



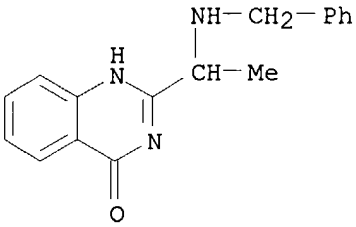
RN 143993-18-4 CAPLUS
CN 4(1H)-Quinazolinone, 2-[1-(butylamino)ethyl]- (9CI) (CA INDEX NAME)



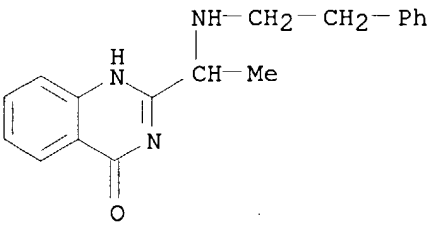
RN 143993-19-5 CAPLUS
CN 4(1H)-Quinazolinone, 2-[1-[(2-hydroxyethyl)amino]ethyl]- (9CI) (CA INDEX NAME)



RN 143993-20-8 CAPLUS
CN 4(1H)-Quinazolinone, 2-[1-[(phenylmethyl)amino]ethyl]- (9CI) (CA INDEX NAME)

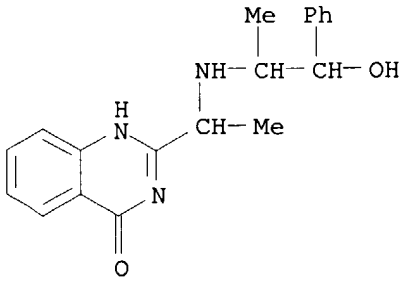


IT **143993-21-9P 143993-22-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 143993-21-9 CAPLUS
CN 4(1H)-Quinazolinone, 2-[1-[(2-phenylethyl)amino]ethyl]- (9CI) (CA INDEX NAME)

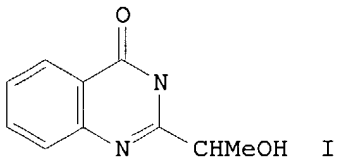


RN 143993-22-0 CAPLUS
CN 4(1H)-Quinazolinone, 2-[1-[(2-hydroxy-1-methyl-2-phenylethyl)amino]ethyl]-

(9CI) (CA INDEX NAME)



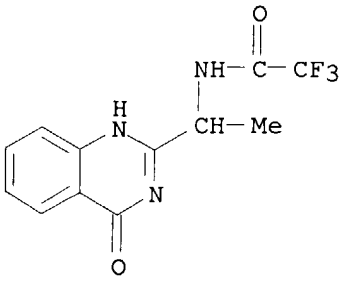
L3 ANSWER 28 OF 30 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1990:571734 CAPLUS
DOCUMENT NUMBER: 113:171734
TITLE: Synthesis of chrysogine, a metabolite of Penicillium chrysogenum and some related 2-substituted 4-(3H)-quinazolinones
AUTHOR(S): Bergman, Jan; Brynolf, Anna
CORPORATE SOURCE: Dep. Org. Chem., R. Inst. Technol., Stockholm, S-100 44, Swed.
SOURCE: Tetrahedron (1990), 46(4), 1295-310
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 113:171734
GI



AB Both enantiomers of chrysogine (I) were prepared from 2-H2NC6H4CONH2 (II). Thus reaction of II and (-)-AcOCHMeCOCl gave (-)-2-AcOCHMeCONHC6H4CONH2 which upon saponification and cyclization induced by aqueous Na2CO3 at room temperature gave (S)-(-)-I. The enantiomeric purity of (S)-(-)-I was determined by NMR. Inversion of (-)-(S)-I using the Mitsunobu reaction, gave (+)-(R)-I. Reduction of 2-acetyl-4(3H)-quinazolinone with bakers' yeast gave (S)-(-)-I. The cyclization method could be extended to a number of 2-(α-hydroxy)alkyl-4-(3H)-quinazolinones.

IT **129768-62-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 129768-62-3 CAPLUS
CN Acetamide, N-[1-(1,4-dihydro-4-oxo-2-quinazolinyl)ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)



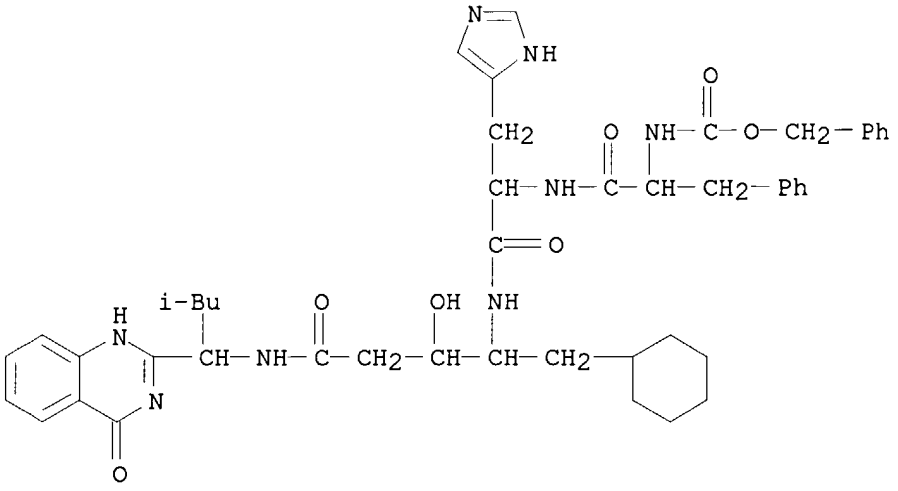
L3 ANSWER 29 OF 30 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1989:135739 CAPLUS
DOCUMENT NUMBER: 110:135739
TITLE: Preparation of 4-amino-3-hydroxy-5-cyclohexylpentanoyl-containing peptides as renin inhibitors
INVENTOR(S): Gante, Joachim; Raddatz, Peter; Sombroek, Johannes; Schmitges, Claus J.; Minck, Klaus Otto
PATENT ASSIGNEE(S): Merck Patent G.m.b.H., Fed. Rep. Ger.
SOURCE: Ger. Offen., 17 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3721855	A1	19880922	DE 1987-3721855	19870702
EP 286813	A2	19881019	EP 1988-102971	19880229
EP 286813	A3	19901212		
R: AT, BE, CH, DE, ES, FR, GB, IT, LI, NL, SE				
AU 8812617	A1	19880915	AU 1988-12617	19880301
AU 614951	B2	19910919		
JP 63258451	A2	19881025	JP 1988-56504	19880311
ZA 8801782	A	19881026	ZA 1988-1782	19880311
HU 49147	A2	19890828	HU 1988-1191	19880311
HU 204848	B	19920228		
PRIORITY APPLN. INFO.:			DE 1987-3707879	19870312
			DE 1987-3721855	19870702

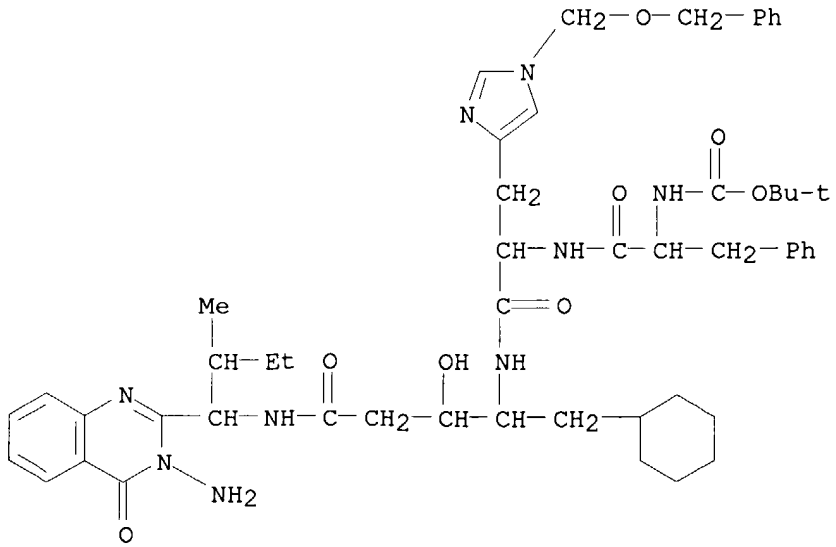
OTHER SOURCE(S): MARPAT 110:135739

AB X-Z-NR2-CHR3-CR4-(CHR5)n-CO-E-NR6-D [I; X = H, R1O(CH2)mCO, R1SO2, etc.; Z = 0-4 amino acid residues chosen from Abu, Ada, Ala, β-Ala, Arg, Asn, Asp, Bia, Cal, Dab, Gln, Glu, Gly, His, N(i.m.)-alkyl-His, Ile, Leu, tert-Leu, Lys, Met, α-Nal, β-Nal, Nbg, Nle, Orn, Phe, Pro, Ser, Thr, Tic, Trp, Tyr, Val; E = 0-2 amino acid residues chosen from Abu, Ala, Cal, His, Ile, Leu, Met, Nle, Phe, Trp, Tyr, Val; D = CH2CH(OH)CH2OH, (CH2)zSO2R7, phenylalkyl, furylalkyl, thienylalkyl, pyridylalkyl, etc.; R1, R3 = H, aryl, arylalkyl, heterocyclyl, heterocyclylalkyl, (substituted) C3-7 cycloalkyl, etc.; R2, R5, R6 = H, alkyl; R4 = :O, (H,OH), (H,NH2); R7 = OH, alkoxy, amino; m = 0-5; n = 1, 2; z = 2-6; Bia = 3-(2-benzimidazolyl)alanyl; Cal = 3-cyclohexylalanyl; Dab = 2,4-diaminobutyryl; α-Nal = α-naphthylalanyl; β-Nal = β-naphthylalanyl, Nbg = (2-norbornyl)glycyl; Tic = tetrahydroisoquinolinyl-1-carbonyl], useful as renin inhibitors (no data), were prepared 2-[1S-(3S-Hydroxy-4S-(N-tert-butoxycarbonylphenylalanylhistidylamino)-5-cyclohexylpentanoylamino)-3-methylbutyl]-3H-quinazolin-4-one was prepared by the solution phase method.

IT **119422-52-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrogenolysis of, in preparation of renin inhibitor)
RN 119422-52-5 CAPLUS
CN L-threo-Pentonamide, 5-cyclohexyl-2,4,5-trideoxy-N-[1-(1,4-dihydro-4-oxo-2-quinazolinyl)-3-methylbutyl]-4-[[N-[N-[(phenylmethoxy)carbonyl]-L-phenylalanyl]-L-histidyl]amino]-, (S)- (9CI) (CA INDEX NAME)

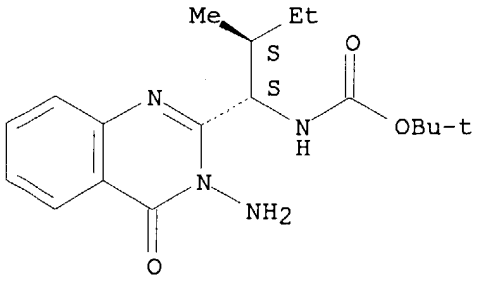


IT **119422-45-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of renin inhibitor)
RN 119422-45-6 CAPLUS
CN L-threo-Pentonamide, N-[1-(3-amino-3,4-dihydro-4-oxo-2-quinazolinyl)-2-methylbutyl]-5-cyclohexyl-2,4,5-trideoxy-4-[[N-[N-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl]-1-[(phenylmethoxy)methyl]-L-histidyl]amino]-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

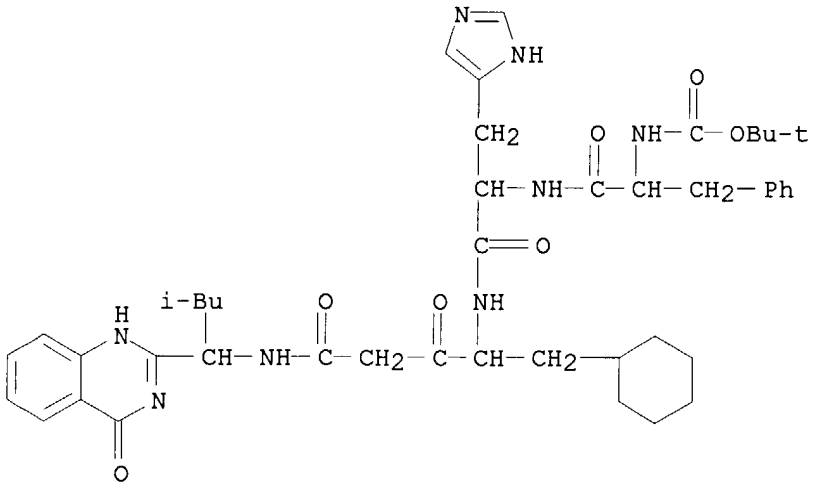


NAME)

Absolute stereochemistry.

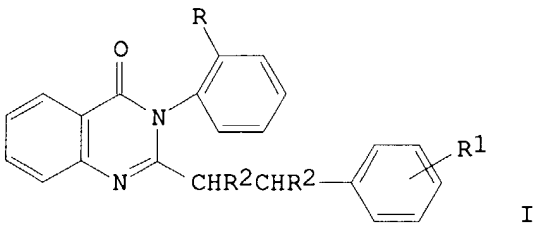


IT **119422-53-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of renin inhibitor)
RN 119422-53-6 CAPLUS
CN L-Histidinamide, N-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-N-[1-(cyclohexylmethyl)-4-[[1-(1,4-dihydro-4-oxo-2-quinazolinyl)-3-methylbutyl]amino]-2,4-dioxobutyl]-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)



L3 ANSWER 30 OF 30 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1985:45864 CAPLUS
DOCUMENT NUMBER: 102:45864
TITLE: Synthesis and antiinflammatory activity of 2-substituted-phenethyl-3-substituted-phenyl-4(3H)-quinazolinones
AUTHOR(S): Singh, Inder Pal; Saxena, A. K.; Sinha, J. N.; Bhargava, K. P.; Shanker, K.
CORPORATE SOURCE: Dep. Pharmacol. Ther., King George's Med. Coll., Lucknow, 226 003, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1984), 23B(6), 592-4
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal

LANGUAGE: English
OTHER SOURCE(S): CASREACT 102:45864
GI



I

AB Quinazolinones I (R = Cl, Me; R1 = 2-OMe, 3-Cl, 2-OH; R2 = N-Phenylpiperazino, homopiperidino, 2-methylpiperidino, morpholino, 4-ClC6H4CH2CH2NH, N(CH2CH2OH)2, piperidino, N-(2-chlorophenyl)piperazino] have been prepared by the bromination of 2-styrylquinazolinones to yield α,β-dibromophenethylquinazolinones which undergo condensation with amines to gives I. 2-(α-Bromo-o,β-dimethoxyphenethyl)-3-(o-chlorophenyl)-4(3H)-quinazolinone has been obtained by the action of MeOH on the dibromo analog. All I show significant antiinflammatory activity. I (R = Cl, R1 = 3-Cl, R2 = N-phenylpiperazino) is the most potent.

IT **94342-55-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antiinflammatory activity of)

RN 94342-55-9 CAPLUS

CN 4(3H)-Quinazolinone, 3-(2-chlorophenyl)-2-[2-(3-chlorophenyl)-1,2-bis[[2-(4-chlorophenyl)ethyl]amino]ethyl]- (9CI) (CA INDEX NAME)